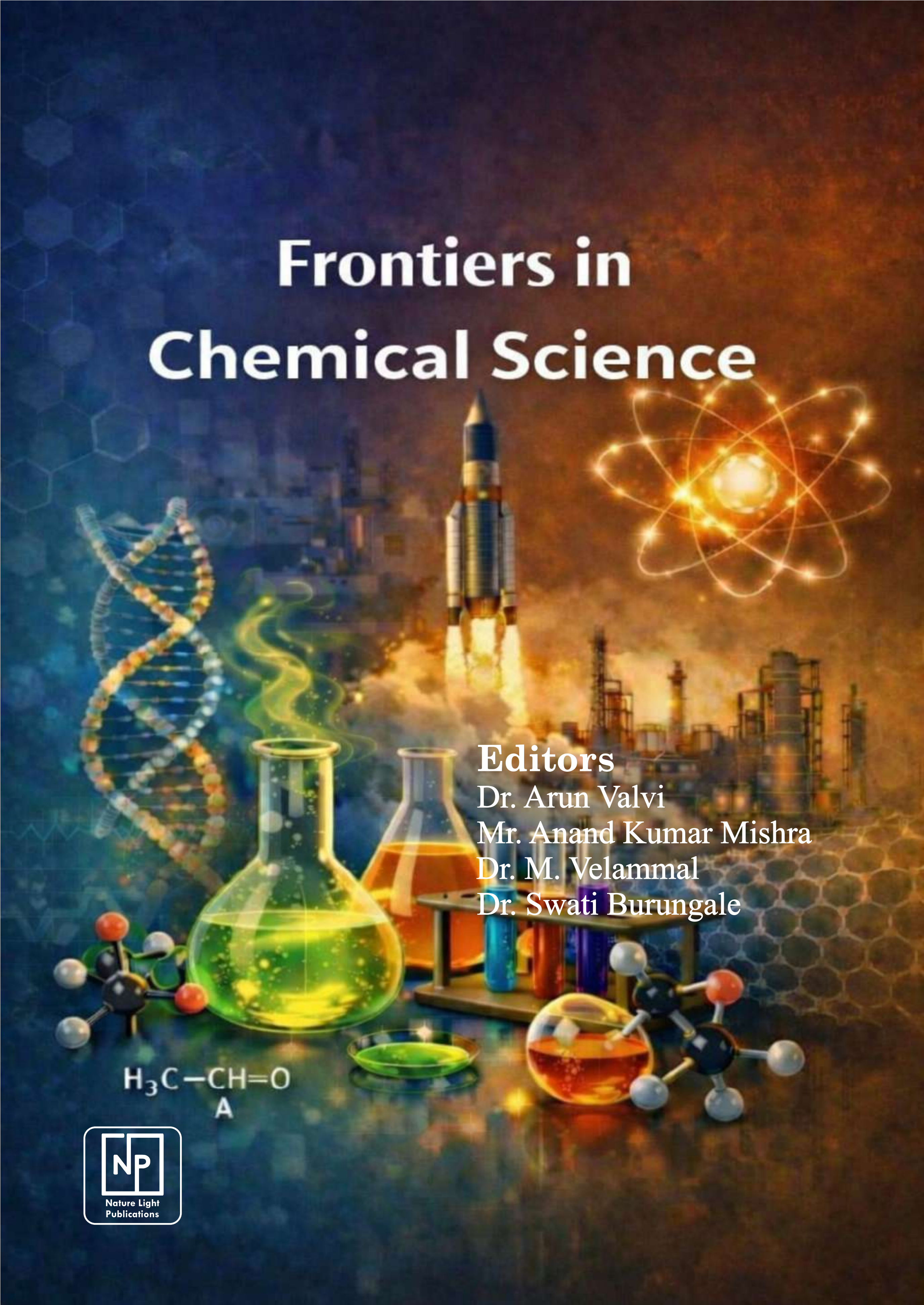
Frontiers in Chemical Science



Editors

Dr. Arun Valvi
Mr. Anand Kumar Mishra
Dr. M. Velammal
Dr. Swati Burungale

NP
Nature Light
Publications

An International Edited Book ISBN-978-93-49938-06-9

FRONTIERS IN CHEMICAL SCIENCE

Editors

Dr. Arun Karansing Valvi
Assistant Professor
Department of Chemistry
Rayat Shikshan Sanstha's Annasaheb
Awate College, Manchar, (MH), India.

Mr. Anand Kumar Mishra
Research Scholar
Department of Chemistry
Deen Dayal Upadhyay Gorakhpur University Gorakhpur, (UP), India.

Dr. M. Velammal
Assistant Professor
NPR College of Engineering and Technology, Tamil Nadu, India.

Dr. Swati Dattatray Burungale
Associate Professor
Delonix Society's Baramati College of Pharmacy,
Barhanpur, Baramati, (MH), India.

Published By

Nature Light Publications

Nature Light Publications, Pune

FRONTIERS IN CHEMICAL SCIENCE

Editors

Dr. Arun Karansing Valvi
Mr. Anand Kumar Mishra
Dr. M. Velammal
Dr. Swati Dattatray Burungale

First Edition: March, 2026

An International Edited Book

ISBN- 978-93-49938-06-9

Published by:
Nature Light Publications, Pune
309 West 11, Manjari VSI Road, Manjari Bk.,
Haveli, Pune- 412 307.
Website: www.naturelightpublications.com
Email: naturelightpublications@gmail.com
Contact No: +91 9822489040 / 9922489040

Preface

The edited volume Frontiers in Chemical Science brings together a diverse and forward-looking collection of research contributions that reflect the dynamic evolution of modern chemistry. As the discipline continues to expand beyond traditional boundaries, it increasingly intersects with materials science, environmental engineering, energy technology, and nanoscience. This book aims to capture these interdisciplinary advancements while providing a platform for emerging ideas, innovative methodologies, and sustainable solutions to global challenges.

The chapters included in this volume highlight significant progress in both fundamental and applied chemical research. A notable focus is placed on environmental remediation and sustainable technologies. The study on the separation of cadmium (II) ions from aqueous solutions using Cyanex 921-based extraction systems demonstrates the importance of advanced separation techniques in addressing heavy metal contamination. Complementing this, research on next-generation graphene derivatives explores their promising role in detoxifying hazardous pollutants from wastewater, emphasizing the growing relevance of nanomaterials in environmental chemistry.

Nanotechnology and advanced materials form another cornerstone of this volume. Contributions on graphene-supported transition metal-doped cadmium sulfide nanocomposites and carbon nanomaterials provide insight into cutting-edge developments in optical properties and energy storage applications. These studies underline the transformative potential of nanostructured materials in revolutionizing electronics, catalysis, and sustainable energy systems.

Energy remains a central theme throughout the book. Chapters on hydrogen production technologies and hydrogen energy systems present comprehensive perspectives on clean fuel alternatives, highlighting both current advancements and future prospects in achieving a low-carbon energy economy. Similarly, the discussion on dye-sensitized solar cells offers valuable *understanding of photovoltaic chemistry, focusing on working principles and reaction kinetics that drive solar energy conversion.*

In addition, the volume addresses innovations in polymer-based hybrid nanocomposites, particularly the development of chitosan/polyvinyl alcohol matrices integrated with green synthesized Al_2O_3–SiO_2 *nanoparticles for food packaging applications. This reflects the increasing importance of sustainable materials in enhancing food safety, shelf life, and environmental compatibility.*

Collectively, the chapters in this book represent a blend of theoretical insights and practical applications, catering to researchers, academicians, and industry professionals. The editors believe that this compilation will not only serve as a valuable academic resource but also inspire further research and collaboration in the ever-evolving field of chemical science.

We extend our sincere gratitude to all contributors for their scholarly efforts and to the reviewers for their valuable feedback. It is our hope that Frontiers in Chemical Science will contribute meaningfully to ongoing scientific discourse and foster innovation for a sustainable and technologically advanced future.

Editors

Frontiers in Chemical Science

Table of Content

Frontiers in Chemical Science

ISBN: 978-93-49938-06-9| Year: 2026 | pp: 01 - 12 |

Separation of Cadmium (II) Ions from Aqueous Solutions using Cyanex 921-Based Extraction System

Rohit Kumar

Jugpal Singh

Pragya Pali

Department of Chemistry, School of Sciences, IFTM University, Lodhipur Rajput, Moradabad (244102), Uttar Pradesh, India

Email: rohit.kumar@iftmuniversity.ac.in

Article DOI Link: https://zenodo.org/uploads/19632701

DOI: 10.5281/zenodo.19632701

Abstract

Cadmium (Cd) is a highly toxic heavy metal released into the environment through industrial activities such as electroplating, battery manufacturing, pigments, and alloy production. Due to its persistence and harmful effects on human health and ecosystems, the removal of Cd(II) ions from aqueous solutions is an important environmental challenge. This chapter focuses on the separation of Cd(II) ions using a Cyanex 921-based extraction system. Cyanex 921 (tri-n-octylphosphine oxide, TOPO) is a neutral organophosphorus extractant known for its strong solvating ability, high chemical stability, and strong affinity toward metal ions in chloride media. The extraction mechanism involves the formation of stable solvated complexes such as $CdCl_2 \cdot 2L$ in the organic phase. Key parameters affecting extraction efficiency, including acidity, chloride concentration, extractant concentration, temperature, and phase ratio, are discussed. Under optimized conditions, Cyanex 921 can achieve extraction efficiencies greater than 99% with high selectivity for Cd(II), making it an effective method for wastewater treatment and metal recovery.

Introduction

Cadmium (Cd) is a highly toxic heavy metal, recognized for its persistence in the environment and its tendency to bioaccumulate in living organisms. Its widespread use in industrial applications—such as battery manufacturing, electroplating, pigments, and alloys—has led to significant environmental contamination, particularly in water bodies. The toxicity of cadmium is well documented: chronic exposure is associated with renal dysfunction, skeletal damage, and possibly carcinogenic effects in humans. Regulatory agencies worldwide, including the World Health Organization (WHO), have established strict limits for cadmium in drinking water. In India, cadmium pollution also raises concern, as the metal accumulates in soft tissues and bones over time, and low-level exposure may lead to long-term health risks. Given these environmental and health risks, removal and recovery of Cd (II) ions (Cd^{2+}) from aqueous solutions are critical objectives in water treatment and industrial waste management. Among the array of available techniques, solvent extraction is particularly attractive because of its high selectivity, efficiency, and adaptability to complex matrices. Specifically, organophosphorus extractants have shown great promise. Among them, Cyanex 921, chemically known as tri-n-octylphosphine oxide (TOPO), has drawn attention due to its excellent chemical stability, strong solvating power, and capacity to form stable complexes with Cd (II) especially in chloride-rich and acidic environments.

Cyanex 921-based systems can be deployed either as liquid–liquid extraction (LLE) or as extractant-impregnated resins (EIRs). These approaches can permit both the removal of cadmium from polluted streams and the recovery of cadmium for reuse, aligning with circular economy goals. The extraction mechanism typically involves coordination between the P=O group of TOPO and cadmium chloride species, forming neutral or partially neutral complexes; research has also elucidated the stoichiometry and thermodynamics of these complexes.

This report provides a comprehensive analysis of the separation of Cd (II) from aqueous solutions using Cyanex 921-based extraction systems. It examines the chemical properties of Cyanex 921, the mechanism and thermodynamics of Cd (II) extraction, the influence of key experimental parameters (e.g., acidity, chloride concentration, extractant concentration, phase ratio), and compares performance with other extractants. The report also discusses environmental considerations, regulatory contexts (with reference to Indian and global standards), and potential industrial applications in wastewater treatment and resource recovery.

Review of Literature

Chemical Nature and Properties of Cyanex 921 (TOPO)

Cyanex 921 chemically known as tri-n-octylphosphine oxide (TOPO), is a neutral, solvating organophosphorus extractant with the molecular formula $C_{24}H_{51}OP$, featuring three long-chain octyl groups attached to a central phosphine oxide moiety and a molecular weight of 386.64 g/mol. It is characterized by a high degree of hydrophobicity, low water solubility and high thermal and chemical stability and is insoluble in water but highly soluble in organic diluents such as kerosene, toluene, and xylene., This configuration imparts high hydrophobicity, low water solubility (approximately 1.1 mg/L in water and 0.2 mg/L in 1 M HCl), and excellent compatibility with hydrocarbon diluents such as kerosene, toluene, and xylene (Choi et al. 2014).

The extractant is a white crystalline solid at room temperature, with a melting point of 50–54°C and a boiling point exceeding 400°C. Its high chemical stability and resistance to hydrolysis make it suitable for repeated extraction and regeneration cycles. Cyanex 921's strong electron-donating P=O group enables it to form stable solvated complexes with metal ions, particularly in the presence of chloride ligands.

Cyanex 921, The key functional group in Cyanex 921 is the phosphoryl (P=O) moiety, which acts as a strong Lewis base, capable of coordinating with metal ions that are soft or borderline acids according to Pearson's Hard–Soft Acid–Base (HSAB) theory. This property underpins its selectivity for metals such as Cd (II), Hg (II), and Ag (I), which exhibit soft acid characteristics.

Speciation of Cd (II) in Chloride Media and Relevant Equilibria

In aqueous chloride solutions, Cd (II) forms a range of chloro-species—Cd^{2+}, $CdCl^{+}$, $CdCl_2^{0}$, $CdCl_3^{-}$, and $CdCl_4^{2-}$—with their relative proportions strongly dependent on $[Cl^{-}]$ (Bazarkina, Zotov, & Akinfiev, 2010; Vanderzee & Irving, 1953). Potentiometric studies show stepwise formation constants for these species, and volumetric data implicates an octahedral-to-tetrahedral structural transition: lower-ligand species (Cd^{2+}, $CdCl^{+}$) are octahedral, while higher-chloride complexes ($CdCl_2^{0}$, $CdCl_3^{-}$, $CdCl_4^{2-}$) adopt tetrahedral coordination (Bazarkina et al., 2010). Spectroscopic evidence using XANES/EXAFS further supports that as chloride concentration increases, Cd's coordination environment shifts from water-rich to chloride-rich (Bazarkina, Zotov, & Akinfiev, 2010). The relevant equilibria can be summarized as:

$$\mathbf{Cd^{2+} + Cl^{-} \rightleftharpoons CdCl^{+}}$$

$$\mathbf{CdCl^{+} + Cl^{-} \rightleftharpoons CdCl_2\ (aq)}$$

$$\mathbf{CdCl_2\ (aq) + Cl^{-} \rightleftharpoons CdCl_3^{-}}$$

$$\mathbf{CdCl_3^{-} + Cl^{-} \rightleftharpoons CdCl_4^{2-}}$$

The predominance of neutral $CdCl_2$ and anionic $CdCl_3^{-}/CdCl_4^{2-}$ species at high chloride concentrations underpins the extraction mechanism by Cyanex 921, which operates via solvation and, to a lesser extent, ion-pair formation.

Extraction Mechanism of Cd (II) by Cyanex 921

Cyanex 921 extracts Cd (II) from chloride media primarily through a solvation mechanism, forming neutral or ion-pair complexes in the organic phase. The general extraction reaction can be represented as:

$$\mathbf{CdCl_2\ (aq) + 2L\ (org) \rightleftharpoons [CdCl_2 \cdot 2L]\ (org)}$$

Where, L denotes Cyanex 921 (TOPO).

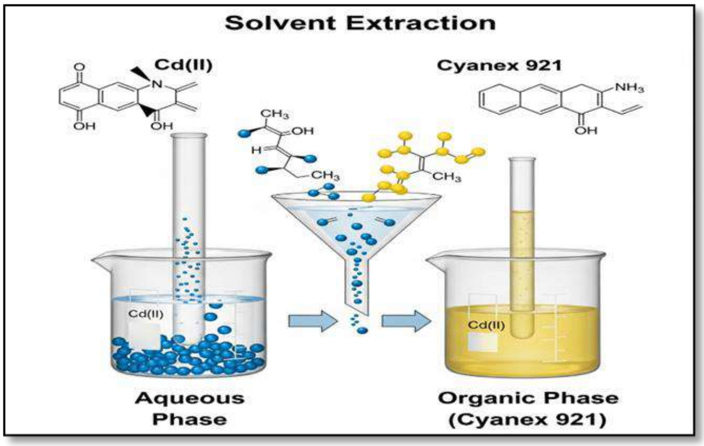


Figure 1: Extraction of Cd (II) by Cyanex 921

For neutral complex formation:

$$\mathbf{CdCl_2\ (aq) + 2TOPO\ (org) \rightleftharpoons CdCl_2{\cdot}2TOPO\ (org)}$$

For ion-pair extraction:

$$\mathbf{CdCl_3^-\ (aq) + H^+\ (aq) + nTOPO\ (org) \rightleftharpoons HCdCl_3{\cdot}nTOPO\ (org)}$$

At higher extractant concentrations, the stoichiometry may shift, with up to four Cyanex 921 molecules coordinating to a single cadmium complex, as evidenced by the formation of [$HCdCl_3{\cdot}4L$] at L concentrations above 0.1 mol/L. The extraction is facilitated by the strong affinity of the P=O group for the cadmium centre, displacing water molecules from the hydration shell and stabilizing the complex in the organic phase (Choi et al. 2014).

Key Experimental Parameters Affecting Extraction

pH and HCl Concentration

The extraction efficiency of Cd (II) by Cyanex 921 is highly sensitive to the acidity and chloride content of the aqueous phase. Optimal extraction occurs in strongly acidic media ($pH < 2$), typically in the range of 1–4 M HCl. At lower acidities, the formation of neutral $CdCl_2$ is favoured, enhancing extraction. However, at very high HCl concentrations (>5 M), the prevalence of highly stable anionic complexes ($CdCl_3^-$, $CdCl_4^{2-}$) can reduce extraction efficiency due to their lower affinity for neutral extractants.

Extractant Concentration and Organic Phase Composition

Increasing the concentration of Cyanex 921 in the organic phase enhances the extraction of Cd (II), with the distribution ratio (D) showing a near-linear relationship with [L] on a log-log scale (slope ≈ 2), indicating the involvement of two extractant molecules per cadmium ion in the predominant complex. The choice of diluent (kerosene, toluene, and xylene) affects phase separation and extraction kinetics, with toluene and kerosene commonly preferred for their low toxicity and good solubility profiles.

Temperature and Thermodynamics

Extraction of Cd (II) by Cyanex 921 is generally exothermic, with increasing temperature leading to a decrease in extraction efficiency. Thermodynamic studies report negative enthalpy changes (ΔH), confirming the exothermic nature of the process. For example, ΔH values of –5.24 J/mol have been reported for Cd (II) extraction by TOPO, with similar trends observed for other neutral organophosphorus extractants.

Phase Ratio (O/A), Contact Time, Mixing, and Kinetics

The organic-to-aqueous (O/A) phase ratio is a critical parameter, influencing both extraction efficiency and phase entrainment. Optimal O/A ratios typically range from 1:1 to 1.5:1, balancing efficient mass transfer with minimal organic carryover. Contact times of 5–10 minutes are generally sufficient to reach equilibrium in well-mixed systems, with faster kinetics observed at higher stirring rates (500–1000 rpm). In EIR systems, equilibrium may require longer contact times (up to 8 hours), particularly at higher metal loadings or lower extractant concentrations.

Stripping/Desorption Conditions and Regeneration

Loaded Cyanex 921 can be efficiently regenerated by stripping the extracted Cd (II) using dilute mineral acids (e.g., 0.1–1 M HNO_3 or HCl) or chelating agents such as EDTA. Stripping efficiencies exceeding 99% have been reported, enabling multiple extraction–stripping cycles with minimal loss of extractant activity.

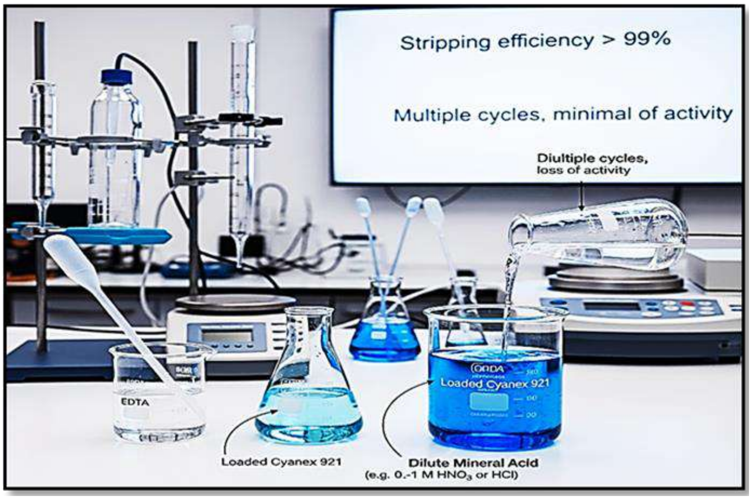


Figure 2: Stripping/Desorption and Regeneration

Supported Systems and Extractant-Impregnated Resins (EIR)

EIRs, prepared by impregnating Amberlite XAD-7 or XAD-4 with Cyanex 921, offer several advantages: high stability of the extractant, ease of handling, and suitability for column operations. Maximum loading capacities of 13–54 mg Cd/g resin have been reported, with equilibrium achieved within 8 hours at 3 M HCl and 366 mg Cyanex 921/g resin. The Langmuir isotherm provides a good fit for sorption data, indicating monolayer adsorption (Navarro et al. 2008).

Methodology

1. Experimental Design & Materials

- **Extractant:** Cyanex 921 (tri-n-octylphosphine oxide, TOPO), purity >93%
- **Supports for EIR:** Amberlite XAD-7 (acrylic polymer, 450 m^2/g surface area) or XAD-4 (styrene-divinyl benzene copolymer, 750 m^2/g)
- **Diluents:** Kerosene, toluene, or xylene
- **Aqueous Phase:** Synthetic or real industrial effluents containing Cd(II), with controlled HCl concentration (0.1–8 M)
- **Other Chemicals:** HNO_3, NaOH, EDTA for stripping and pH adjustment

Preparation of Extractant-Impregnated Resin (EIR)

- **Conditioning:** Amberlite XAD-7/XAD-4 is washed with ketone and nitric acid to remove impurities and then dried.
- **Impregnation:** The resin is contacted with a solution of Cyanex 921 in ketone (0.5 M) for 24 hours under agitation.
- **Solvent Removal:** The mixture is evaporated under reduced pressure to immobilize Cyanex 921 on the resin.
- **Quantification:** The amount of extractant loaded is determined by mass difference after methanol extraction and drying.

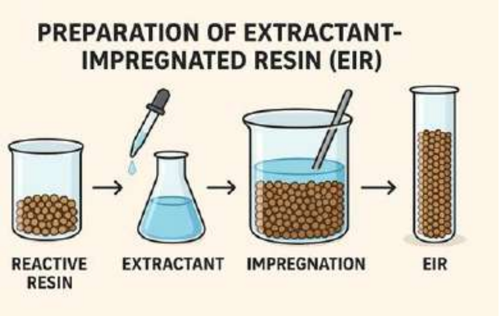


Figure 3: Preparation of Extractant-Impregnated Resin (EIR)

Liquid-Liquid Extraction Procedure

- **Preparation of Solutions:** Aqueous solutions of Cd (II) (10–100 mg/L) are prepared in varying HCl concentrations (0.1–8 M).

- **Extraction:** Equal volumes of aqueous and organic phases (O/A = 1:1, unless otherwise specified) are mixed in a separatory funnel or batch reactor.
- **Mixing:** The mixture is agitated at 500–1000 rpm for 5–30 minutes at controlled temperature (20–60°C).
- **Phase Separation:** After settling, the aqueous and organic phases are separated for analysis (Rydberg et al., 2004; Singh et al., 2010; Darwish & El-Reefy, 2012).

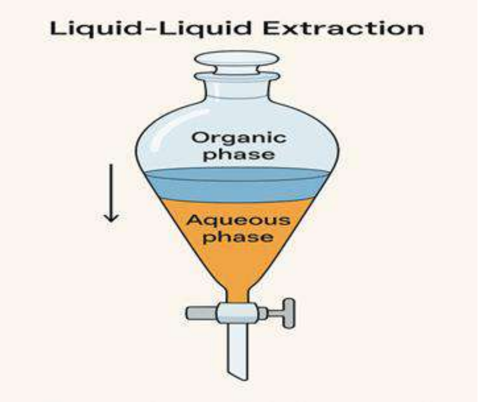


Figure 4: Liquid-Liquid Extraction

Sorption Experiments (EIR)

- **Kinetics:** Samples are withdrawn at intervals to monitor Cd (II) uptake over time.
- **Isotherms:** Experiments are conducted at varying initial Cd (II) concentrations to construct adsorption isotherms.

Figure 5: Sorption Experiment

Stripping and Regeneration

- **Stripping:** Loaded organic or resin phases are contacted with 0.1–1 M HNO_3, HCl, or EDTA solutions.

- **Regeneration:** The extractant or resin is washed and reused for subsequent extraction cycles.

Data Analysis

- **Distribution Ratio (D):** D = [Cd]org / [Cd]aq
- **Extraction Efficiency (%E):** %E = 100 × D / (O/A + D)
- **Isotherm Modelling:** Langmuir and Freundlich models for adsorption data
- **Thermodynamics:** Calculation of ΔH, ΔS, and ΔG from temperature-dependent data

Environmental and Safety Assessment

- **Toxicity and Solubility:** Evaluation of extractant loss and effluent composition.
- **Regulatory Compliance:** Monitoring of residual Cd (II) and extractant in treated water.

Expected Outcomes

Extraction Efficiency and Selectivity

- **High Extraction Efficiency:** Cyanex 921 achieves >99% extraction of Cd (II) from 2–4 M HCl solutions at 0.3 mol/L extractant concentration and O/A ratio of 1–1.5 within 10 minutes.
- **Stoichiometry:** Predominant extracted species are [$CdCl_2 \cdot 2L$] and [$HCdCl_3 \cdot 4L$], depending on extractant concentration.
- **Selectivity:** Cyanex 921 demonstrates high selectivity for Cd (II) over Ni (II), Zn (II), Fe (III), Cu (II), and Pb (II), particularly in multi-component solutions simulating battery leachates or electroplating effluents.

Influence of Experimental Parameters

- **pH and HCl Concentration:** Optimal extraction at pH < 2 and 2–4 M HCl. Extraction decreases at very high acidities due to stabilization of anionic Cd complexes.
- **Extractant Concentration:** Extraction efficiency increases with [Cyanex 921], with two extractant molecules per Cd (II) ion.
- **Temperature:** Extraction is exothermic; increasing temperature reduces efficiency ($\Delta H \approx -5$ to -44 kJ/mol).
- **Phase Ratio and Contact Time:** O/A ratios of 1–1.5 and contact times of 5–10 minutes are optimal for LLE; EIR systems may require longer contact times (up to 8 hours).
- **Mixing:** Higher stirring rates accelerate equilibrium attainment and improve phase separation.

Stripping and Regeneration

- Stripping Efficiency: >99% of Cd (II) can be stripped from loaded organic or resin phases using 0.1–1 M HNO_3 or HCl.
- Regeneration: Cyanex 921 and EIRs retain >90% of their extraction capacity over multiple cycles (up to 15 cycles reported).

Supported Systems (EIR)

- **Loading Capacity:** Maximum sorption capacities of 13–54 mg Cd/g resin, depending on extractant loading and HCl concentration.
- **Isotherm Fit:** Langmuir model provides a good fit, indicating monolayer adsorption.
- **Kinetics:** Pseudo-second-order kinetics dominates, with equilibrium reached within 8 hours.

Process Design and Scale-Up

- **Stage Requirements:** Two counter-current stages are sufficient for quantitative extraction (>99.9%) of Cd (II) at optimized conditions.
- **Stripping:** Three-stage counter-current stripping achieves >99% recovery of Cd (II).
- **Phase Entrainment:** Optimal O/A ratios (1–1.5) minimize organic carryover and maximize extraction efficiency.

Environmental and Safety Outcomes

- **Effluent Quality:** Treated water meets or exceeds regulatory limits for cadmium.
- **Extractant Loss:** Low aqueous solubility of Cyanex 921 minimizes environmental release.
- **Toxicity:** Cyanex 921 is of moderate hazard; proper handling and waste management are required (Safarzadeh et al. 2007; Chemical Book 2024)

Analytical Monitoring

- **Detection Limits:** AAS and ICP-OES provide detection limits in the low µg/L range, suitable for process control and regulatory compliance.
- **Speciation:** Chloride ion-selective electrodes and back titration enable monitoring of Cd (II) speciation and extraction equilibria.

Recent Advances

- **Alternative Extractants:** Ionic liquids and biosorbents are being explored for enhanced selectivity and sustainability, but Cyanex 921 remains a benchmark for industrial-scale applications.

- **Process Integration:** Cyanex 921-based extraction can be integrated with electrowinning or precipitation for complete metal recovery (Adigun et al. 2024; John et al. 2025)

Conclusion

The separation of Cd (II) ions from aqueous solutions using Cyanex 921-based extraction systems represents a mature and highly effective approach for addressing the dual challenges of environmental protection and resource recovery. The chemical principles underlying the process—anchored in the solvation of neutral and anionic cadmium chloro-complexes—enable high selectivity and efficiency, even in the presence of competing metal ions.

Key advantages of Cyanex 921 include

- High Extraction Efficiency: Achieving >99% removal of Cd(II) under optimized conditions.
- Operational Flexibility: Effective in both liquid-liquid and solid-phase (EIR) systems.
- Selectivity: Superior discrimination against common co-contaminants (Ni, Zn, Fe, Cu, Pb).
- Regeneration and Reusability: Robust performance over multiple extraction–stripping cycles.
- Environmental Compatibility: Low aqueous solubility and moderate toxicity reduce environmental risks.
- Industrial Applicability: Proven effectiveness in battery recycling, electroplating effluent treatment, and other hydrometallurgical processes.

Environmental and regulatory compliance is readily achievable, with treated effluents meeting stringent standards for cadmium content. The process also aligns with circular economy principles, enabling the recovery and reuse of valuable metals from waste streams.

Future directions include the integration of Cyanex 921-based extraction with advanced process control, the exploration of hybrid systems (e.g., supported liquid membranes, ionic liquids), and the continued refinement of extractant formulations for enhanced sustainability.

In conclusion, Cyanex 921-based extraction systems offer a scientifically robust, operationally flexible, and environmentally responsible solution for the selective separation of cadmium from aqueous solutions, supporting both industrial productivity and environmental stewardship.

References

1. Institute of Medicine. (1995). Case study 6: Cadmium toxicity. In Environmental Medicine: Integrating a Missing Element into Medical Education (pp. 231–235). The National Academies Press.

2. Leopold, A. A., Coll, M. T., Fortuny, A., & Sastre, A. M. (2014). Liquid-liquid extraction of Cd (II) from pure and Ni/Cd acidic chloride media using Cyanex 921: a selective treatment of hazardous leachate of spent Ni–Cd batteries. Journal of Hazardous Materials, 201–202, 18–25.
3. World Health Organization. (2022). Cadmium – Chemical fact sheet. In Guidelines for Drinking-water Quality, 4th edition (2022 update).
4. Choi, S.-Y., Nguyen, V. T., Lee, J.-C., Kang, H., & Pandey, B. D. (2014). Liquid–liquid extraction of Cd(II) from pure and Ni/Cd acidic chloride media using Cyanex 921: A selective treatment of hazardous leachate of spent Ni–Cd batteries. Journal of Hazardous Materials, 278, 258–266.
5. Bazarkina, E. F., Zotov, A. V., & Akinfiev, N. N. (2010). Pressure-dependent stability of cadmium chloride complexes: Potentiometric measurements at 1–1000 bar and 25 °C. Geology of Ore Deposits, 52(2), 167-178.
6. Bazarkina, E. F., Zotov, A. V., & Akinfiev, N. N. (2010). Structure and stability of cadmium chloride complexes in hydrothermal fluids. Chemical Geology, 276(1–2), 1-17.
7. Vanderzee, C. E., & Irving, H. (1953). The stability constants of cadmium chloride complexes: Variation with temperature and ionic strength. Journal of the American Chemical Society, 75(22), 5927-5931.
8. Mazarakioti, E. C., Angelone, M., Ruggiero, B., & Pashalidis, I. (2019). Modeling the solvent extraction of cadmium (II) from aqueous chloride media. Molecules, 24(22), 4178.
9. Navarro, R., Saucedo, I., Núñez, A., Ávila, M., & Guibal, E. (2008). Cadmium extraction from hydrochloric acid solutions using Amberlite XAD-7 impregnated with Cyanex 921 (tri-octyl phosphine oxide). Reactive and Functional Polymers, 68(2), 557-571.
10. Rydberg, J., Cox, M., Musikas, C., & Choppin, G. R. (2004). Solvent Extraction Principles and Practice (2nd ed.). Marcel Dekker, New York.
11. Singh, D. K., Mishra, S., & Tripathi, V. S. (2010). Solvent extraction of cadmium from chloride media using Cyanex 921. Separation and Purification Technology, 75(2), 152–157.
12. Darwish, M. S., & El-Reefy, S. A. (2012). Solvent extraction of cadmium (II) from hydrochloric acid solutions using organophosphorus extractants. Hydrometallurgy, 113–114, 45–51.
13. Safarzadeh, M., Bafghi, M. Sh., Moradkhani, D., & Ojaghi-Ilkhchi, M. (2007). A review on hydrometallurgical extraction and recovery of cadmium from various resources. Minerals Engineering, 20(5), 435-444.
14. Chemical Book. (n.d.). Cyanex 921 (tri-n-octyl-phosphine oxide) – risk & safety information. Retrieved August 14, 2024, from https://www.chembk.com/en/chem/CYANEX%20921

15. Adigun, B., Thapaliya, B. P., Luo, H., & Dai, S. (2024). Ionic liquid-based extraction of metal ions via polymer inclusion membranes: a critical review. RSC Sustainability, 2, 2768–2780. https://doi.org/10.1039/D4SU00297K
16. John, G., & co-authors. (2025). Adsorption and recovery studies of cadmium and lead ions using biowaste adsorbents from aqueous solution. Separations, 12(1), 16. https://doi.org/10.3390/separations1201001

Frontiers in Chemical Science

ISBN: 978-93-49938-06-9| Year: 2026 | pp: 13 - 25 |

Next-Generation Graphene Supported Transition Metal Doped Cadmium Sulfide Nanocomposites, for Advanced Optical Properties and Energy Storage Applications

[1]Dr. Dorothy S

[2]Ms. Jeevitha R

[3]Ms. Srimathi M

[1]Assistant Professor, Department of Chemistry, AMET University, Chennai, India.

[2,3]Research scholar, Department of Chemistry, AMET University, Chennai, India

Email: dorothys@ametuniv.ac.in

Article DOI Link: https://zenodo.org/uploads/19632881

DOI: 10.5281/zenodo.19632881

Abstract

In this chapter the graphene-based transition metal doped cadmium sulfide (CdS) nanocomposites represent a bright and potential type of advanced materials to be used in the next generation optical and energy storage devices. It provides an overview on the design, synthesis and properties of this hybrid material. CdS is a semiconductor with wide-band-gap, which is highly efficient, optically transparent with tunable optoelectronics, the practical functionality is often limited by spontaneous charge recombination and photo-corrosion. The addition of graphene or reduced graphene oxide (rGO) can significantly improve the charge transportation, surface area as well as structural stability. Besides, transition metal doping (Cu, Co, or Fe) creates defect states that help separate charge more easily and create a longer wavelength and optical absorption. The role of the dopants in tailoring the band structure, the reduction of particle size, and the improvement of the electron-hole dynamics are paid special attention. Their performance in electrochemical properties will prove their applications in high-efficiency energy storage systems like batteries, supercapacitors and the increased photocatalytic absorption. Altogether this graphene-based transition metal doped cadmium sulfide (CdS) nanocomposites investigated for a flexible material platform, which provides numerous improvements to the energy conversion and storage technology, as well as sustainable material design.

Keywords: Cadmium Sulfide (CdS), Transition metals, graphene, reduced graphene oxide (rGO), electrochemical application.

Introduction

In the past decades the most prominent research field in modern science are nanoscience and nanotechnology, these phenomena occurring in systems with nanometer dimensions, sized between 1 to 100 nanometers. It is the study of manipulating matter on an atomic and molecular scale, they also deal with design, fabrication, application of nanostructures or nanomaterials, that the fundamental understanding of the relationships between physical properties and material dimensions. Many new materials developed in this size are able to create devices with a vast range of applications, such as in medicines, electronics, biomaterials and energy production have unique properties compared with their bulk materials. Among different nanoparticles, semiconductor materials have attracted a lot of attention, such as cadmium sulfide (CdS)(1), Zinc oxide (ZnO)(2), Titanium dioxide (TiO2) (3) have excellent energy storage, catalytic and optical properties. CdS nanoparticles is one of the significant chalcogenide materials because of size dependent, availability of discrete energy levels, tunable bandgap, developed a synthetic protocol, easy preparation technique, with good chemical stability and optical properties (4). Preparation of CdS nanocomposite it is quite difficult to control their particle size. Consequently, to control the size of the CdS Np's and to enhance their properties, the supporting carbon material, reduced graphene oxide (rGO) is a promising material because of its high stability, surface area, mechanical strength, kinetics, and electron transfer (5). Transition metal ions doped into the semiconductor nanoparticles have been widely investigated in recent years because of its unusual changes in their properties. By tuning the optical, electrical and magnetic properties of some nanostructures by varying their sizes, morphology and structures has been extensively studied (6),(7). Specifically, transition metal such as iron (Fe), Cobalt (Co), and Copper (Cu) are doped to the composite materials. The main objective of this chapter, discuss about the graphene supported transition metal doped cadmium sulfide nanocomposites, fabrication method of the composites and its electrochemical and photocatalytic application.

Materials

1. Semiconductor Nanomaterial: Cadmium Sulfide

One of the widely studied II-VI semiconductor materials is cadmium sulfide, has excellent optoelectronic characteristics (8). The crystallized form of CdS is mostly in the form of two structures namely the hexagonal Wurtzite and the Cubic Zn-blende structure. Wurtzite is thermodynamically stable at normal conditions but the Zinc-blende is common in particles that are of nanoscale (9). CdS nanoparticles has direct band gap of (2.42 eV), enabling it to be effectively absorbed in the visible light hence making it a good material to be used in photocatalysis and converting to solar energy. They have various desirable attributes, which has high absorption coefficients, photoconductivity and tunable electronic properties. These characteristics allowed the CdS to multiple applications such as photodetectors, light-emitting devices, solar cells, gas sensors and photocatalysts. Nevertheless, CdS is usually impractical due to rapid recombination of the photogenerated charge carriers, as well as because of photocorrosion (10).To overcome these limitations, researchers have dwelt into alternative measures like heterostructure formation, surface modification and doping with the use of transition metals. Transition-metal doping has been one of these methods, and has become a potent means of collective control of the electronic structure and enhancement of the performance of CdS-based nanomaterials.

2. Supporting Materials with Graphene and Reduced Graphene Oxide

Graphene is a two-dimensional notable carbon compound that comprises a layer of planar hybridized (sp2) carbon atoms in a hexagonal configuration. Geim and Novoselov experimental discovery and isolation in 2004 have given unimaginable publicity to graphene since then because of its remarkable physical and chemical characteristics. It possesses high thermal conductivity (11), mechanical strength (12), excellent electrical conductivity (13), and high specific surface area.

Graphene oxide is a derivative of graphene that has been oxidized with various oxygen functional groups, such as carboxyl, epoxy, and hydroxyl groups among others. These functional groups help in the dispersion of GO to aqueous media and offer active sites where nanoparticles are to be attached. GO may be reduced in chemicals or thermally to result in reduced graphene oxide that removes the devastated p-electron network, and increases electrical conductivity.

Materials made of graphene are popular supporting matrices of semiconductor nanoparticles. Due to the high surface area of the admitted sheets of graphene, nanoparticles can be dispersed evenly, avoiding agglomeration to enhance stability. Further, graphene is a good electron acceptor and transporter and thus facilitates easy separation of charges as well as minimizes recombination process of photo generated carriers. All these properties contribute to the optical, catalytic, and electrochemical functions of graphene-based nanocomposites to high material.

3. Transition Metal Doping in CdS/Graphene Composites

A few of the transition metals have been explored as dopants in CdS nanoparticles and they include copper, cobalt, nickel, manganese, and iron. Dorothy et al., 2024, studied copper-doped CdS nanoparticles are found to be better conductive electrically and more electrochemical active because of the number of extra charge carriers introduced (14) Likewise, cobalt doping is also possible to manipulate the magnetic and optical characteristics of CdS and is therefore applicable to spintronic and optoelectronic operation. Iron doping has been noticed to influence photocatalytic activity accelerating charge separation and absorbing more visible light (15).

When transition-metal doping is used in combination with graphene support, these nanocomposites exhibit significantly improved optical and electrochemical characteristics, and these results are highly efficient. These materials tested to have good potential uses in energy storage and environmental influences.

Nanomaterials Synthesis Methods and Properties

Synthesis and processing of nanomaterials and nanostructures are the essential aspect of nanotechnology. Studies on new physical, chemical properties and applications of nanomaterials or nanostructures are possible only when nanostructured materials are made available with desired size, morphology, crystal and microstructure and chemical composition. There are two approaches to the synthesis of nanomaterials and the fabrication of nanoparticles,

- Top-down
- Bottom-up

1. Top-Down Approach

To obtain the nanosized particle, a block of a bulk material is whittled or sculpted, i.e., breaking down the bulk material into smaller and smaller dimensions. The top-down approach includes Milling or Attrition and Lithography techniques. The surface structure's imperfections are the main issue with the top-down approach. It is well known that traditional top-down methods, like lithography, can seriously harm the processed patterns' crystallography and even introduce new flaws during the etching process. For instance, lithographically produced nanowires are not smooth and may have numerous impurities and surface structural flaws. Since nanostructures and nanomaterials haves have a very high surface to volume ratio, such flaws would have a substantial effect on their physical characteristics and surface chemistry. Because of the inelastic surface scattering caused by the surface imperfection, conductivity would be decreased, resulting in excessive heat generation and additional. Top-down methods will continue to be crucial in the synthesis and production of nanostructures and nanomaterials; despite the surface flaws and other flaws they may introduce.

2. Bottom-Up Approach

Although bottom-up approaches are not new in material synthesis, they are frequently highlighted in the literature on nanotechnology. Typical material synthesis, which has been used in industry for more than a century, involves building materials atom by atom on a very large scale. Examples include the growth of single crystals, the deposition of films, and the chemical industry's production of salt and nitrate, and in the electronics sector. As long as the material in question has the same chemical composition, crystallinity, and microstructure, most materials have the same physical characteristics regardless of the synthesis methods used.

Naturally, for kinetic reasons, distinct synthesis and processing techniques frequently produce noticeable variations in the material's chemical composition, crystallinity, and microstructure. As a result, the material has various physical characteristics.

3. Preparation of Graphene - Supported CdS Nanocomposite via Co-precipitation

Different method of synthesis has been formulated on how to prepare transition metal doped graphene-supported CdS nanocomposites. These techniques include co-precipitation, hydrothermal synthesis (16), solvothermal techniques and reflux techniques. Co-precipitation is a feasible technique through doping semiconductor nanoparticles by using transition metals to alter the electronic structure of the nanoparticles and improve the functionality of the nanoparticles. It is very easy, cost-effective and it can be used to generate uniform nanoparticles. Transition metals like Fe, Co, Cu doped CdS/rGO composite materials were prepared by ease and simple co-precipitation method by one-pot synthesis process starting from GO (Graphite Oxide) to rGO (Reduced Graphene Oxide).

In a standard synthesis protocol, the modified Hummers method is used in the preparation of graphene oxide starting with the graphite powder. Ultra-sonication is subsequently used to disperse the GO sheets in an appropriate solvent to have a stable colloidal suspension. To the dispersion metal precursors, which include cadmium acetate and transition-metal salts, are introduced, and a sulfur source which may include thiourea is then added. The reaction proceeds by the formation of a hybrid nanocomposite on the surface of graphene sheets penetrated by the CdS nanoparticles. Inclusion of transition metal ions in CdS lattice causes the introduction of localized states of energy between the band gap. Such defect states are capable of existing as a charge carrier trapping center thus, suppressing electron-hole recombination enhancing photocatalytic activity.

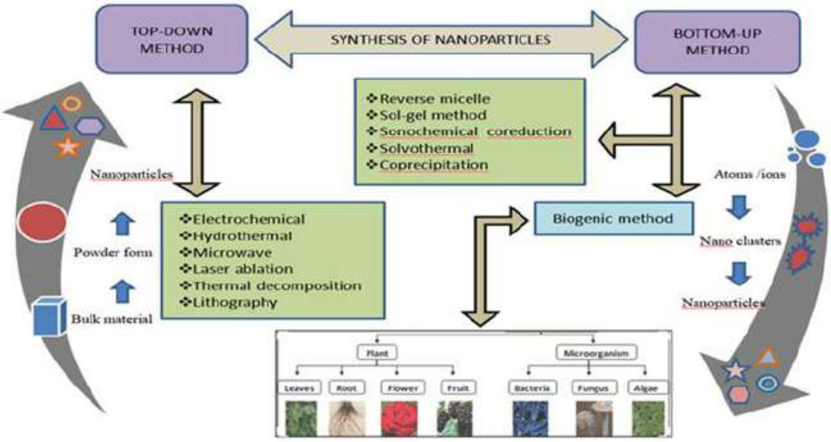


Figure 1.1 Nanoparticles synthesis methods

It has been established that the morphology of, as well as the size of the particles CdS, occurs in the presence of graphene in a very large degree. The transmission electron microscopy images indicate that CdS nanoparticles are evenly dispersed on the surface of the graphene, making it easy not to form aggregates and thus improving stability. The resulting nanocomposites are found to be better in electrical conductivity and electrochemical activity than pure CdS nanoparticles.

4. Properties of Nanomaterials

When materials are reduced to the nanoscale, their properties can differ from those at the macro scale, allowing for novel applications. The energy band structure and charge carrier density in the materials can be modified quite differently from their bulk counterpart and in turn will modify the electronic and optical properties of the materials.

The mechanical properties of the nanomaterials are varied like the hardness, elastic modulus, fracture toughness, scratch resistance and fatigue strength etc. The Chemical properties of nanoparticles can be discussed in terms of enhanced reactivity and catalytic activity. For thermal properties, small particles may be incorporated better in base matrix (e.g. without reducing strength) and provide better thermal conduction.

The electrical resistivity of nano-crystalline materials is expected to be higher than that of the corresponding coarse-grained polycrystalline ones due to the increased volume fraction of the atoms lying on the grain boundaries. The absorption or emission wavelength can be controlled by size selection, as it was seen that semiconductors like CdS, ZnS, and ZnSe exhibits blue shifts as particle size decreases. The decrease of the particle size to the nano-range results often in improved magnetic behavior (as compared to their bulk counterparts). Nanoparticles present a higher surface to volume ratio with decreasing size of nanoparticles. The properties of nanomaterials have been shown in the figure 1.2.

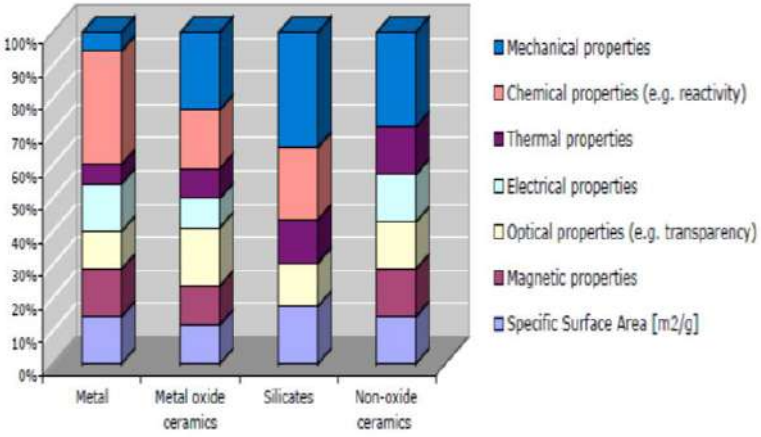


Figure 1.2 Properties of Nanomaterials

CdS nanoparticles can display novel optical, electronic, magnetic, chemical and structural properties that might find many important technological applications. Optically active metal dopants, which can be adjusted to modify the material's optical, luminescence, or magnetic properties, are one way to modify the intrinsic electronic characteristics of II-IV semiconductors without altering the particle size (17). The characteristics of CdS nano particles can be modified to some useful extent by doping with Co, Ni and other metal ions. The important properties of CdS are shown in Table 1.1.

Table 1.1 Properties of CdS

Molecular Formula	**CdS**
Molar Mass	144.48 g/mol
Appearance	Yellow – orange to brown solid
Density	4.82 g/cm^3
Crystal structure	Cubic, Hexagonal
Specific heat	0.47 J/gK
Thermal conductivity at (25°C)	0.2 W/cmK
Melting point	1750°C, 2023 K, 3182° F (10 MPa)
Boiling point	980°C, 1253 K, 1796° F (subl.)
Lattice parameter at 300 K	a = 0.4135 nm, c = 0.6749 nm
Static dielectric constant	8.9
Refractive index (n_D)	2.52
Energy gap	2.42 eV, direct
Exciton binding energy	28 meV

Application of Nanoparticles

Currently nanotechnology is described as revolutionary discipline in terms of its possible impact on industrial applications. Nanotechnology offers potential solutions to many problems using emerging nano-techniques, depending on the strong interdisciplinary character of nanotechnology there are many research fields and several potential applications that involve nanotechnology. Nanoparticles are employed to improve existing products, which brings a revolutionary change in the areas such as biomedicine, chemistry, energy storage, information and communication sector, industrial sector, electronics, fuel cell, etc. the schematic diagram of nanotechnology applications is shown in Figure 1.3.

Figure 1.3 Applications of nanotechnology

1. Optical Characterization Structural Characterization

Extensive methods of characterization are used in order to study the structural, morphological, and optical properties of graphene-focused CdS nanocomposites. The structure of the crystal and phase composition of the produced materials is usually determined with the use of X-ray diffraction (XRD) analysis. The formations of the cubic zinc-blende or hexagonal wurtzite structure of CdS nanoparticles are usually validated by the diffraction patterns.

Fourier transform infrared spectroscopy (FTIR) can give the information on the functional groups in graphene oxide and reduced graphene oxide. Reduction and disappearance of oxygen containing functional groups prove the success of the process of transformation GO to rGO. further displays the structural characteristic of graphene using the characteristic D and G bands as obtained by Raman spectroscopy.

The morphology and size distribution of the particle sizes of the nanocomposites are analyzed under the electron microscopy techniques which include scanning electron microscopy (SEM), and the transmission electron microscopy (TEM). The results of these analyses usually indicate the existence of smooth CdS nanoparticles suspended on the sheets of graphene of size 2-10 nm. The dispersion of nanoparticles on the graphene surface is a contributing factor towards the increased catalytic and electrochemical activity.

2. Electrochemical and Energy storage

The potential of graphene-based CdS nanocomposites containing more than 20 elements has demonstrated great potential in energy storage systems like the supercapacitors, as well as, lithium-ion batteries. Graphene has a high electrical conductivity that allows the quick transportation of electrons, whereas the CdS nanoparticles offer active sites of electrochemical reactions.

Electrochemical analysis of cyclic voltammetry has revealed that the transition metal doped CdS/rGO samples have a high degree of current density than pure CdS nanoparticles. Introduction of transition-metal dopant improves the electrochemical activity through the improvement of the rate of charge transfer and the active sites. Moreover, the high surface area composites made of graphene have adsorbent capacitance of better electrolyte ions to enhance capacitance and energy density. The mentioned properties render graphene based CdS nanocomposites as potentially very promising in the prospect of energy storage in the next generation.

Besides being used as an energy storage system, CdS nanocomposites anchored on graphene have also proved to be excellent photocatalysts to be used in environmental remedial efforts (18). These substances have a capacity to ozone organic pollutants and dyes visible-irradiation. The increased photocatalytic effects are attributed to visual photogenerated charge carrier separation with the help of the graphene network.

It has been reported in the recent studies that iron-doped CdS/GO nanocomposites have a high photocatalytic degradation efficiency when compared with CdS (undoped). Defect states induced with the presence of Fe ions enhance the process of charge carrier separation and high absorption of visible light. Consequently, high degradation efficiencies of such toxic dyes as methyl orange in the presence of the sun may be attained with the use of these materials (14). Similarly, ZnO doped CdS/GO nanocomposites were compared to binary ZnO/CdS composites, pure ZnO, and bare CdS, to enhance the photocatalytic and photoelectrochemical activity of ternary nanocomposite.

Future Prospects and Advances

Although there have been a lot of advances with regards to the fabrication of graphene-based transition metal doped CdS nanocomposites, there are more challenges that need to be overcome. The toxicity of cadmium-based materials is one of the biggest concerns and this may be deadly on the environment and health. Subsequent studies ought to work on upgrading the stability and recyclability of these materials without causing much pollutant to the environment.

The other significant issue is the mass production of graphene-based nanocomposites of controlled morphology and composition. The ability to make these materials cost effective and scalable will attract significant effort to commercialize these materials in the field of energy and environmental benefit.

The combination of computational modeling, machine learning, and experimental strategies in the future can potentially be used to design ultraoptimal nanocomposites of the next generation with rational design. Such interdisciplinary directions will hasten the production of high-performance materials in technological energy sustainable applications.

Conclusion

In summary the graphene-based transition metal doped cadmium sulfide (CdS) nanocomposites represent an alternative promising multifunctional material with a significant potential of enhanced optical and energy storage properties. The integration of CdS nanoparticles on graphene-based substrates is one way to overcome the inherent limitations of undoped CdS by enhancing charge separation, increases structure stability and reducing recombination. Doping transition metals such as Cu, Co, and Fe plays a vital role in tuning the electronic band structure creating defects and enhancing the visible light absorption, significantly enhancing optical and electrochemical properties. This chapter has considered the design, synthesis, optical and electrochemical activities has been focused. The nanocomposites they are obtained are shown better in further functionalities such as a photocatalysis and energy storage system because they have high surface area, increased conductivity, and effective charge transport mechanisms. However, there are still the difficulties related to the scale, high stability and ecological impact that cadmium-based materials have to be addressed. Future research is to maintain the desirable properties of these nanocomposites by sustainable pathways towards synthesis, increased optimization, concentrations of dopants and alternative non-toxic components. Overall, these future hybrid materials offer solid framework to realize the evolution of the energy technologies and environmental solutions.

References

1. M. Danish, A. Ashraf, Z.A. Sandhu, M.A. Raza, A.H. Bhalli, A.G. Al-Sehemi, Electrochemical studies of CdS based nanocomposite: Synthesis, characterization and structural aspects insight, J. Mol. Struct. 1294 (2023). https://doi.org/10.1016/j.molstruc.2023.136296.
2. A.N. Ghoti, A.B. Patil, S.K. Pardeshi, ZnO/CdS heterostructure embellished rGO nanosheet for photocatalytic hydrogen generation and photoelectrochemical performance, Mater. Chem. Phys. Sustain. Energy 4 (2025) 100031. https://doi.org/10.1016/j.macse.2025.100031.
3. Q. Chen, M. Zhang, J. Li, G. Zhang, Y. Xin, C. Chai, Construction of immobilized 0D/1D heterostructure photocatalyst Au/CuS/CdS/TiO2 NBs with enhanced photocatalytic activity towards moxifloxacin degradation, Chem. Eng. J. 389 (2020). https://doi.org/10.1016/j.cej.2020.124476.
4. F. Antolini, M. Pentimalli, T. Di Luccio, R. Terzi, M. Schioppa, M. Re, L. Mirenghi, L. Tapfer, Structural characterization of CdS nanoparticles grown in polystyrene matrix by thermolytic synthesis, Mater. Lett. 59 (2005) 3181–3187. https://doi.org/10.1016/j.matlet.2005.05.047.
5. W. Han, L. Ren, L. Gong, X. Qi, Y. Liu, L. Yang, X. Wei, J. Zhong, Self-assembled three-dimensional graphene-based aerogel with embedded multifarious functional nanoparticles and its excellent photoelectrochemical activities, ACS Sustain. Chem. Eng. 2 (2014) 741–748. https://doi.org/10.1021/sc400417u.

6. X. Chen, S.S. Mao, Titanium dioxide nanomaterials: Synthesis, properties, modifications and applications, Chem. Rev. 107 (2007) 2891–2959. https://doi.org/10.1021/cr0500535.
7. M. Ni, M.K.H. Leung, D.Y.C. Leung, K. Sumathy, A review and recent developments in photocatalytic water-splitting using TiO2 for hydrogen production, Renew. Sustain. Energy Rev. 11 (2007) 401–425. https://doi.org/10.1016/j.rser.2005.01.009.
8. V. Singh, P.K. Sharma, P. Chauhan, Synthesis of CdS nanoparticles with enhanced optical properties, Mater. Charact. 62 (2011) 43–52. https://doi.org/10.1016/j.matchar.2010.10.009.
9. H.M. Saleh, A.I. Hassan, Synthesis and Characterization of Nanomaterials for Application in Cost-Effective Electrochemical Devices, Sustain. 15 (2023). https://doi.org/10.3390/su151410891.
10. R. Bhattacharya, S. Saha, Growth of CdS nanoparticles by chemical method and its characterization, Pramana - J. Phys. 71 (2008) 187–192. https://doi.org/10.1007/s12043-008-0152-7.
11. S. Kaveri, L. Thirugnanam, M. Dutta, J. Ramasamy, N. Fukata, Thiourea assisted one-pot easy synthesis of CdS/rGO composite by the wet chemical method: Structural, optical, and photocatalytic properties, Ceram. Int. 39 (2013) 9207–9214. https://doi.org/10.1016/j.ceramint.2013.05.025.
12. D. Li, M.B. Müller, S. Gilje, R.B. Kaner, G.G. Wallace, Processable aqueous dispersions of graphene nanosheets, Nat. Nanotechnol. 3 (2008) 101–105. https://doi.org/10.1038/nnano.2007.451.
13. F. Liu, S. Song, D. Xue, H. Zhang, Folded structured graphene paper for high performance electrode materials, Adv. Mater. 24 (2012) 1089–1094. https://doi.org/10.1002/adma.201104691.
14. A. Razaq, F. Bibi, X. Zheng, R. Papadakis, S.H.M. Jafri, H. Li, Review on Graphene-, Graphene Oxide-, Reduced Graphene Oxide-Based Flexible Composites: From Fabrication to Applications, Mater. 2022, Vol. 15, 15 (2022). https://doi.org/10.3390/ma15031012.
15. C. Li, Z. Wei, Y. Chen, L. Ma, S. Huang, L. Li, J. Ma, Photo-electrochemical and enhanced photocatalytic activity of CdS/rGO nanocomposites prepared by hydrothermal method, J. Mater. Sci. Mater. Electron. 32 (2021) 22093–22105. https://doi.org/10.1007/s10854-021-06679-8.
16. S. Dorothy, T. Lavanya, K. Punithamurthy, R. Jayavel, K. Satheesh, Optical Characterization and Electrochemical Properties of Cd(1−x)Cu(x)S/rGO Composites Synthesized Through Reflux Method, J. Nanosci. Nanotechnol. 16 (2016) 9716–9721. https://doi.org/10.1166/jnn.2016.12078.
17. S. Dorothy, P. Sugumar, S. Meenakshi, M. Settu, S. Devanesan, K. Kalpana, S. Dixit, K. Rajendran, Iron-Doped Cadmium Sulfide/Graphene Oxide (Cd(1-

x)Fe(x)S/GO) Nanocomposites for Photocatalytic Degradation of Toxic Pollutants, Luminescence 39 (2024). https://doi.org/10.1002/bio.70044.

18. A. Parihar, P. Sharma, N.K. Choudhary, R. Khan, A. Gupta, R.K. Sen, H.C. Prasad, M. Ashiq, Green Synthesis of CdS and CdS/rGO Nanocomposites: Evaluation of Electrochemical, Antimicrobial, and Photocatalytic Properties, ACS Appl. Bio Mater. 6 (2023) 3706–3716. https://doi.org/10.1021/acsabm.3c00390.
19. S. Sagadevan, Z.Z. Chowdhury, M.R. Bin Johan, F.A. Aziz, L.S. Roselin, H.L. Hsu, R. Selvin, Synthesis, characterization and electrochemical properties of cadmium sulfide – Reduced graphene oxide nanocomposites, Results Phys. 12 (2019) 878–885. https://doi.org/10.1016/j.rinp.2018.12.058.
20. R. Murugan, A. Rebekah, J.A. Allen, M. Preethi, C. Viswanathan, N. Ponpandian, Engineering the semiconducting CdS nanostructures by N-doped rGO to enhance the adsorption sites: Promising electrocatalyst to hydrogen evolution reaction Int. J. Hydrogen Energy 47 (2022) 1610616120. https://doi.org/10.1016/j.ijhydene.2022.03.129.
21. Z. Yin, M. Li, N. Wang, Z. Zhou, Y. Hu, D. Fan, Y. Pang, Y. Liu, Z. Lu, J. Hai, CdS and ZnS deposition on rGO via. an emulsion-solvothermal method through direct deposition to achieve a high photocatalytic activity and stability, Appl. Surf. Sci. 612 (2023) 155844. doi.org/10.1016/j.apsZ. https://doi.org/10.1016/j.apsusc.2022.155844.
22. R.P. Nikam, A.C. Lokhande, S.D. Khot, V.J. Mane, C.D. Lokhande, Chemical synthesis and photoelectrochemical study of CdS/rGO nanocomposite films, J. Korean Ceram. Soc. 2022 602 60 (2022) 238–251. https://doi.org/10.1007/s43207-022-00258-1.
23. Ö. Uğuz, Ö. Budak, A. Koca, Simultaneous electrodeposition of electrochemically reduced graphene oxide-binary metal chalcogenide composites to enhance photoelectrochemical performance, Int. J. Hydrogen Energy 46 (2021) 35290–35301. https://doi.org/10.1016/j.ijhydene.2021.08.064.
24. A. Thakur, P. Thakur, S. Baccar, Structural Properties of Nanoparticles, Integr. Nanomater. Their Appl. (2023) 57–80. https://doi.org/10.1007/978-981-99-6105-4_4.
25. Y.R. Smith, R. Gakhar, A. Merwin, S.K. Mohanty, D. Chidambaram, M. Misra, Anodic titania nanotube arrays sensitized with mn- or co-doped cds nanocrystals, Electrochim. Acta 135 (2014) 503–512. https://doi.org/10.1016/j.electacta.2014.05.005.
26. D.B. Pal, A.K. Rathoure, A. Singh, Investigation of surface interaction in rGO-CdS photocatalyst for hydrogen production: An insight from XPS studies, Int. J. Hydrogen Energy 46 (2021) 26757–26769. https://doi.org/10.1016/j.ijhydene.2021.05.173.

27. A. Ghasempour, H. Dehghan, M. Ataee, B. Chen, Z. Zhao, M. Sedighi, X. Guo, M.A. Shahbazi, Cadmium Sulfide Nanoparticles: Preparation, Characterization, and Biomedical Applications, Mol. 2023, Vol. 28, 28 (2023). https://doi.org/10.3390/molecules28093857.
28. K. Liu, B. Du, L. Zhao, Y. Lei, Y. Wang, C. Li, L. Luo, Y. Deng, Z. Tang, J. Chen, Preparation and properties of CdS0.25Se0.75/N-GQDs/3D rGO ternary composites, J. Mater. Sci. Mater. Electron. 2024 3518 35 (2024) 1226-. https://doi.org/10.1007/s10854-024-12913-w.
29. H. Alijani, M. Abdouss, H. Khataei, Efficient photocatalytic degradation of toxic dyes over BiFeO3/CdS/rGO nanocomposite under visible light irradiation, Diam. Relat. Mater. 122 (2022) 108817. https://doi.org/10.1016/j.diamond.2021.108817.
30. C. Yuan, H. Lv, Y. Zhang, Q. Fei, D. Xiao, H. Yin, Z. Lu, Y. Zhang, Three-dimensional nanoporous heterojunction of CdS/np-rGO for highly efficient photocatalytic hydrogen evolution under visible light, Carbon N. Y. 206 (2023) 237–245. https://doi.org/10.1016/j.carbon.2023.02.022.

Frontiers in Chemical Science

ISBN: 978-93-49938-06-9| Year: 2026 | pp: 26 - 30 |

Hydrogen Production Technologies

[1]Immanuel Prabaharan S

[2]Dr. Muthurajan S

[1]Research Scholar, Department of EEE, AMET University, Chennai

[2]Assistant Professor, Department of Marine Engineering, AMET University, Chennai

Email: imman.amet@gmail.com

Article DOI Link: https://zenodo.org/uploads/19632954

DOI: 10.5281/zenodo.19632954

Abstract

Hydrogen is widely regarded as a clean and sustainable energy carrier with the potential to decarbonize multiple sectors, including transportation, industry, and power generation. As global energy demand rises and environmental concerns intensify, hydrogen production technologies have gained significant attention. This chapter presents a comprehensive overview of conventional and emerging hydrogen production methods, including thermochemical, electrochemical, biological, and photolytic processes. It highlights key techniques such as steam methane reforming (SMR), water electrolysis, biomass gasification, and photoelectrochemical splitting. The chapter also examines efficiency, cost, environmental impact, and scalability of different technologies. Emerging innovations such as green hydrogen, artificial photosynthesis, and carbon capture integration are discussed. Finally, the chapter outlines challenges and future directions for sustainable hydrogen production.

Keywords: Hydrogen production, green hydrogen, electrolysis, steam methane reforming, biomass gasification, renewable energy, fuel cells, clean energy

Introduction

The global energy sector is undergoing a transformation toward cleaner and more sustainable sources. Hydrogen has emerged as a promising energy carrier due to its high energy density and zero carbon emissions at the point of use. It can be used in fuel cells, industrial processes, and energy storage systems.

Currently, most hydrogen is produced from fossil fuels, leading to significant carbon emissions. Therefore, there is an urgent need to develop sustainable hydrogen production technologies. This chapter explores various hydrogen production methods and evaluates their potential for large-scale adoption.

Classification of Hydrogen Production Technologies

Hydrogen production technologies can be broadly categorized into
- Thermochemical methods
- Electrochemical methods
- Biological methods
- Photolytic methods

Each method differs in terms of energy source, efficiency, cost, and environmental impact.

Thermochemical Hydrogen Production

1. Steam Methane Reforming (SMR)

SMR is the most widely used method for hydrogen production.

Process

Methane reacts with steam at high temperatures (700–1000°C) to produce hydrogen and carbon monoxide.

Advantages
- High efficiency
- Mature technology

Limitations
- High CO_2 emissions
- Dependence on fossil fuels

2. Coal Gasification

Coal reacts with oxygen and steam to produce syngas ($CO + H_2$).

Challenges
- High carbon emissions
- Environmental concerns

3. Biomass Gasification

Biomass is converted into hydrogen-rich gas through thermochemical processes.

Benefits
- Renewable source
- Lower carbon footprint

Electrochemical Hydrogen Production

1. Water Electrolysis

Electrolysis splits water into hydrogen and oxygen using electricity.

Types

- Alkaline electrolysis
- Proton Exchange Membrane (PEM) electrolysis
- Solid Oxide Electrolysis (SOE)

Advantages

- Produces high-purity hydrogen
- Can use renewable energy (solar, wind)

Limitations

- High cost of electricity
- Infrastructure requirements

Biological Hydrogen Production

1. Bio-Photolysis

Microorganisms use sunlight to split water into hydrogen.

2. Dark Fermentation

Organic substrates are converted into hydrogen by anaerobic bacteria.

3. Photo-Fermentation

Photosynthetic bacteria produce hydrogen using light and organic compounds.

Advantages

- Eco-friendly
- Utilizes waste materials

Challenges

- Low efficiency
- Scalability issues

Photolytic Hydrogen Production

1. Photoelectrochemical (PEC) Water Splitting

Uses semiconductor materials and sunlight to produce hydrogen.

2. Artificial Photosynthesis

Mimics natural photosynthesis to generate hydrogen using solar energy.

Benefits

- Renewable and sustainable
- Zero emissions

Limitations

Technology still under development

Green Hydrogen and Sustainability

Green hydrogen is produced using renewable energy sources such as solar and wind through electrolysis. It is considered the most sustainable form of hydrogen.

Advantages

- Zero carbon emissions
- Supports energy transition

Challenges

- High production cost
- Limited infrastructure

Integration with Carbon Capture and Storage (CCS)

Blue hydrogen combines fossil-based production with carbon capture technologies to reduce emissions. CCS plays a crucial role in minimizing environmental impact.

Applications of Hydrogen

- Fuel cells for transportation
- Power generation
- Industrial processes (ammonia, steel production)
- Energy storage systems

Challenges in Hydrogen Production

- High cost of green hydrogen
- Storage and transportation issues
- Infrastructure limitations
- Energy efficiency concerns

Future Perspectives

Future research directions include

- Development of cost-effective catalysts
- Scaling up renewable electrolysis systems
- Integration with smart grids
- Advances in hydrogen storage technologies

Conclusion

Hydrogen production technologies are central to the transition toward a sustainable energy future. While traditional methods dominate current production, emerging technologies offer cleaner alternatives. Green hydrogen, powered by renewable energy, holds the greatest promise for reducing carbon emissions. However, challenges related to cost, efficiency, and infrastructure must be addressed.

Continued innovation and policy support will be essential to unlock the full potential of hydrogen as a clean energy carrier.

References

1. John A. Turner, Gail Sverdrup, and Mark K. Mann (2024). Hydrogen production pathways and future prospects. International Journal of Hydrogen Energy, 49(5), 2150–2165.
2. Martin Ball and Martin Wietschel (2025). The future of hydrogen – opportunities and challenges. Energy Policy, 185, 113500.
3. Xiaohong Wang, Yongdan Li, and Jian Liu (2024). Advances in water electrolysis for hydrogen production. Renewable Energy, 210, 1200–1215.
4. Anil Kumar, Sanjay Kumar Singh, and Ravi Prakash (2025). Biomass gasification for hydrogen production: A review. Bioresource Technology, 380, 129200.
5. James R. McKone, Nathan S. Lewis, and Harry B. Gray (2024). Artificial photosynthesis for sustainable hydrogen production. Chemical Reviews, 124(3), 1456–1500.
6. Dmitri Bessarabov, Helena Wang, and Haijiang Li (2025). PEM electrolysis systems for green hydrogen production. Journal of Power Sources, 610, 233500.
7. Rakesh Sharma, Priya Verma, and Amit Gupta (2025). Biological hydrogen production technologies: Current status and future prospects. Biotechnology Advances, 72, 108350.
8. Yonghua Li, Qiang Zhang, and Zhenyu Chen (2024). Photoelectrochemical water splitting for hydrogen production. Nano Energy, 110, 108300.

Frontiers in Chemical Science

ISBN: 978-93-49938-06-9| Year: 2026 | pp: 31 - 40 |

Hydrogen Energy System

[1]Aswini M

[2]S. Muthurajan

[1]Research Scholar, Department of Electrical and Electronics Engineering, AMET University, Kanathur, Chennai-603112

[2]Assistant Professor, Department of Marine Engineering, AMET University, Kanathur, Chennai-603112

Email: aswinifalls@gmail.com

Article DOI Link: https://zenodo.org/uploads/19633089

DOI: 10.5281/zenodo.19633089

Abstract

Hydrogen energy systems have gained significant attention as a sustainable solution to address the growing global energy demand and environmental concerns associated with fossil fuel consumption. As a clean and versatile energy carrier, hydrogen offers the potential to reduce greenhouse gas emissions and support the transition toward a low-carbon energy economy. This chapter presents a comprehensive overview of hydrogen energy systems, focusing on their fundamental principles, production methods, storage technologies, and utilization strategies. The discussion begins with the basic concept of hydrogen as an energy carrier, emphasizing its high energy content and environmental benefits. Various hydrogen production methods, including steam methane reforming, electrolysis, and biomass-based processes, are examined with respect to efficiency, cost, and environmental impact. The chapter further explores different storage techniques such as compressed gas, liquid hydrogen, and solid-state storage, highlighting the challenges associated with hydrogen's low volumetric density and safety considerations.

In addition, the utilization of hydrogen in fuel cells for power generation and transportation applications is discussed, along with its role in industrial processes and renewable energy integration. The ability of hydrogen to act as an energy storage medium for intermittent renewable sources is also analyzed, demonstrating its importance in improving energy reliability and grid stability. Despite its advantages, challenges such as high production costs, infrastructure limitations, and technological constraints are addressed. Finally, the chapter outlines future trends in

hydrogen energy, including advancements in green hydrogen production, fuel cell technologies, and global investments in hydrogen infrastructure. Overall, this chapter provides a theoretical foundation for understanding hydrogen energy systems and their potential to contribute to sustainable and energy-efficient solutions in modern energy applications.

Introduction

The increasing global demand for energy, combined with the adverse environmental effects of fossil fuel consumption, has created an urgent need for alternative and sustainable energy sources. Fossil fuels such as coal, oil, and natural gas have been the primary sources of energy for decades; however, their continued use has led to significant environmental problems, including air pollution, global warming, and climate change. As a result, there is a growing emphasis on developing clean and renewable energy technologies that can reduce dependence on fossil fuels and minimize environmental impact.

Hydrogen has emerged as a promising energy carrier due to its unique properties and environmental benefits. It is the most abundant element in the universe and can be produced from a variety of resources, including water, natural gas, and biomass. When used in energy systems, hydrogen produces only water as a by-product, making it an environmentally friendly alternative to conventional fuels. Furthermore, hydrogen can be stored and transported, allowing it to serve as a link between energy production and consumption.

Hydrogen energy systems encompass the entire process of hydrogen production, storage, distribution, and utilization. These systems are designed to convert primary energy sources into hydrogen, store it efficiently, and use it for various applications such as electricity generation, transportation, and industrial processes. The development of hydrogen energy systems is therefore essential for achieving a sustainable and energy-efficient future.

Fundamentals of Hydrogen Energy

Hydrogen is not a primary energy source but an energy carrier, meaning that it must be produced using energy from other sources. This characteristic distinguishes hydrogen from fossil fuels and highlights its role in energy systems as a medium for storing and transporting energy. One of the most significant advantages of hydrogen is its high energy content per unit mass, which is nearly three times higher than that of gasoline. This makes hydrogen particularly attractive for applications where weight is a critical factor, such as transportation.

However, hydrogen also presents certain challenges due to its physical properties. It has a very low density under standard conditions, which makes storage and transportation difficult. To overcome this issue, hydrogen must be compressed, liquefied, or stored in specialized materials. These processes require additional energy and infrastructure, which can affect the overall efficiency of hydrogen energy systems.

The conversion of hydrogen into usable energy typically occurs through electrochemical processes, such as those in fuel cells. In a fuel cell, hydrogen reacts with oxygen to produce electricity, heat, and water. This process is highly efficient and does not involve combustion, resulting in lower emissions and higher energy efficiency compared to traditional energy conversion methods

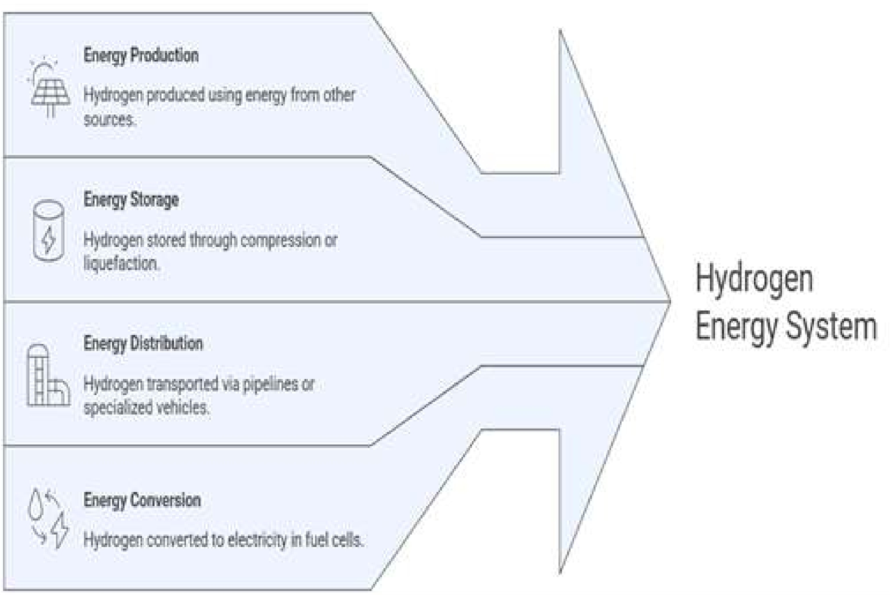


Figure 1: Basic Hydrogen Energy System Flow

Hydrogen Production Methods

Hydrogen can be produced through a variety of methods, each with its own advantages, limitations, and environmental impacts. The most widely used method is steam methane reforming (SMR), which involves reacting natural gas with steam to produce hydrogen and carbon dioxide. Although SMR is cost-effective and well-established, it is not environmentally sustainable due to the emission of greenhouse gases.

Electrolysis of water is considered a cleaner method of hydrogen production, especially when powered by renewable energy sources. In this process, electricity is used to split water into hydrogen and oxygen. When renewable energy sources such as solar or wind are used, the resulting hydrogen is referred to as “green hydrogen,” which has minimal environmental impact. However, the high cost and energy requirements of electrolysis remain significant challenges.

Other methods of hydrogen production include biomass gasification and thermochemical processes. Biomass gasification involves converting organic materials into hydrogen through high-temperature reactions, while thermochemical processes use heat and chemical reactions to produce hydrogen. These methods offer potential for sustainable hydrogen production but require further development to become economically viable.

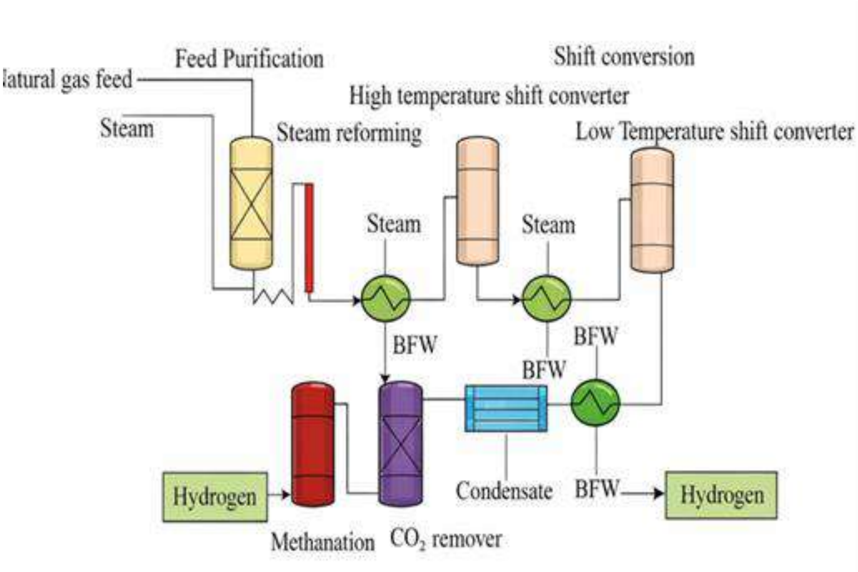


Figure 2: Hydrogen Production Methods

Hydrogen Storage Technologies

Hydrogen storage is one of the most critical and challenging aspects of hydrogen energy systems, as it directly influences the efficiency, safety, and practicality of hydrogen utilization. Due to its extremely low density under ambient conditions, hydrogen requires advanced storage methods to achieve sufficient energy density for real-world applications. The selection of an appropriate storage technique depends on factors such as application requirements, cost, safety considerations, and energy efficiency. Broadly, hydrogen storage technologies can be classified into three main categories: compressed gas storage, liquid hydrogen storage, and solid-state storage.

Compressed gas storage is the most widely used and commercially available method for storing hydrogen. In this approach, hydrogen is stored at high pressures, typically ranging from 350 to 700 bar, in specially designed high-strength cylinders made from composite materials. This method is relatively simple and allows for fast charging and discharging, making it suitable for applications such as hydrogen fuel cell vehicles. However, the need for high-pressure containment systems increases the cost and raises safety concerns, as any leakage or structural failure can lead to hazardous situations. Additionally, the energy required for compressing hydrogen reduces the overall system efficiency.

Liquid hydrogen storage involves cooling hydrogen to extremely low temperatures, around −253°C, to convert it into a liquid state. In this form, hydrogen achieves a much higher energy density compared to compressed gas, making it suitable for applications where space is limited, such as aerospace and large-scale energy systems. However, the liquefaction process is highly energy-intensive and requires sophisticated cryogenic storage tanks with excellent insulation. Moreover, boil-off losses, where a portion of the liquid hydrogen gradually evaporates, present a challenge for long-term storage and transportation.

Solid-state storage methods represent an emerging and promising area of hydrogen storage technology. In this approach, hydrogen is stored within solid materials such as metal hydrides, chemical hydrides, or porous materials like carbon nanotubes and metal-organic frameworks. These materials absorb hydrogen at the molecular level, allowing for higher storage densities and improved safety compared to gaseous or liquid storage. Solid-state storage systems operate at lower pressures and temperatures, reducing the risks associated with high-pressure or cryogenic systems. However, challenges such as slow hydrogen absorption and release rates, high material costs, and limited storage capacity currently restrict their widespread adoption.

In addition to these primary storage methods, ongoing research is focused on developing advanced hybrid storage systems that combine the advantages of different techniques. Innovations in materials science, nanotechnology, and system design are expected to improve storage efficiency, reduce costs, and enhance safety. Effective hydrogen storage is essential for enabling the large-scale deployment of hydrogen energy systems, as it directly impacts transportation, distribution, and end-use applications. As technology continues to evolve, advancements in hydrogen storage will play a crucial role in the success of the hydrogen economy.

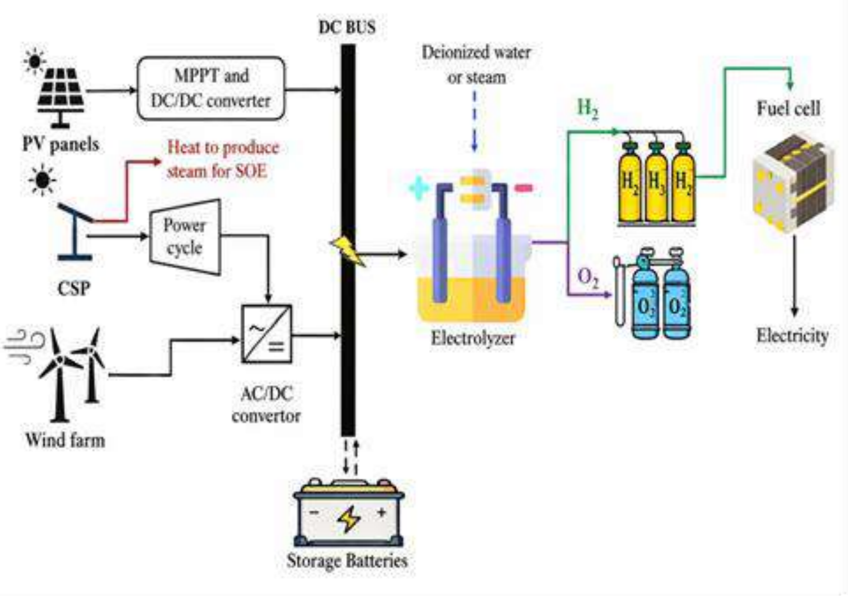


Figure 3: Hydrogen Storage Methods

Hydrogen Utilization and Applications

Hydrogen can be utilized in a wide range of applications, making it a versatile energy carrier. One of the most important applications is in fuel cells, which convert hydrogen into electricity through an electrochemical process. Fuel cells are highly efficient and produce zero emissions, making them suitable for both stationary and mobile applications.

In the transportation sector, hydrogen is used as a fuel for fuel cell vehicles (FCVs), which offer an alternative to conventional internal combustion engine vehicles. These vehicles produce only water as an emission, significantly reducing air pollution. Hydrogen is also used in industrial processes, such as refining and chemical production, where it serves as a key raw material.

In addition, hydrogen plays a crucial role in energy storage, particularly in renewable energy systems. Excess energy generated from renewable sources can be used to produce hydrogen, which can be stored and later converted back into electricity when needed. This capability enhances the reliability and stability of energy systems.

Integration with Renewable Energy Systems

The integration of hydrogen energy systems with renewable energy sources plays a crucial role in achieving a sustainable and reliable energy infrastructure. Renewable energy sources such as solar and wind are inherently intermittent, meaning their power generation depends on environmental conditions like sunlight and wind speed. This variability creates challenges in maintaining a continuous and stable energy supply. Hydrogen offers an effective solution to this problem by acting as an energy storage medium that can store excess energy generated during peak production periods and release it when demand exceeds supply.

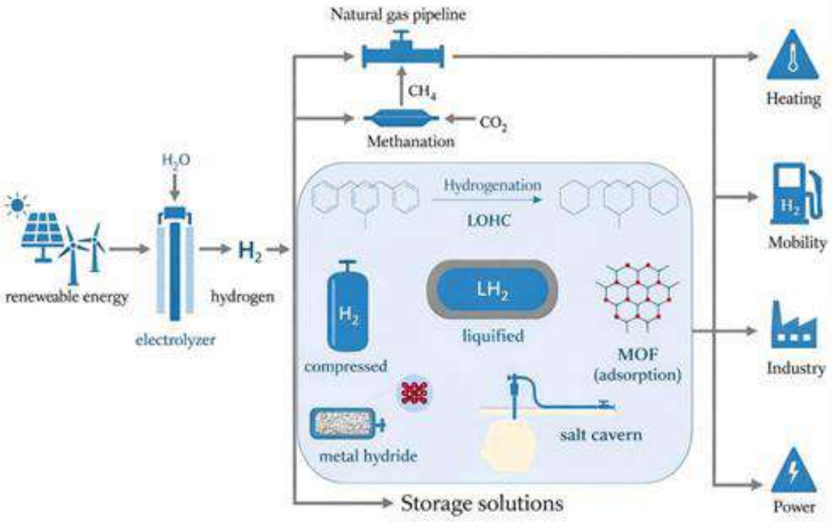


Figure 4: Renewable Energy Integrated Hydrogen System

During periods of high renewable energy generation, surplus electricity that cannot be immediately used or stored in conventional batteries can be utilized for hydrogen production through electrolysis. In this process, electrical energy is used to split water into hydrogen and oxygen, effectively converting electrical energy into chemical energy stored in hydrogen. The produced hydrogen can then be stored for long durations without significant losses, making it suitable for seasonal energy storage. When energy demand increases or renewable generation decreases, the stored hydrogen can be converted back into electricity using fuel cells or combustion systems, thereby ensuring a stable energy supply.

Furthermore, the integration of hydrogen systems with renewable energy contributes to grid flexibility and resilience. Hydrogen can be transported and distributed across different locations, enabling decentralized energy systems and reducing dependence on centralized power plants. This approach supports the development of smart grids and energy networks that can efficiently manage energy resources. In addition, hydrogen integration helps in reducing curtailment losses, where excess renewable energy is otherwise wasted due to limited storage capacity. As a result, hydrogen serves as a key enabler for maximizing the utilization of renewable energy and facilitating the transition toward a low-carbon and sustainable energy ecosystem.

Challenges in Hydrogen Energy Systems

Hydrogen energy systems, despite their significant potential, face several technical and economic challenges that limit their widespread adoption. One of the primary challenges is the high cost associated with hydrogen production, particularly for green hydrogen generated through electrolysis using renewable energy. The efficiency of current electrolysis technologies is still limited, and the dependence on expensive renewable infrastructure increases the overall cost. In addition, conventional production methods such as steam methane reforming, although cost-effective, result in carbon emissions, which contradict the goal of sustainability.

Another major challenge is hydrogen storage and transportation. Due to its low volumetric energy density, hydrogen requires high-pressure compression, liquefaction at extremely low temperatures, or advanced material-based storage techniques. These methods not only increase the complexity of storage systems but also raise safety concerns, as hydrogen is highly flammable and requires strict handling protocols. Furthermore, the lack of a well-developed hydrogen distribution infrastructure poses a significant barrier to large-scale implementation.

Infrastructure and technological limitations also contribute to the challenges in hydrogen energy systems. The absence of widespread refueling stations, pipelines, and storage facilities restricts the practical use of hydrogen, especially in transportation applications. Additionally, issues related to durability and lifespan of fuel cells, along with the need for rare and expensive materials such as platinum catalysts, further complicate system development. Addressing these challenges requires coordinated efforts in research, policy-making, and industrial investment.

Future Trends in Hydrogen Energy

The future of hydrogen energy systems is highly promising, driven by advancements in technology and increasing global emphasis on clean energy solutions. One of the most significant trends is the rapid development of green hydrogen, which is produced using renewable energy sources such as solar and wind. As the cost of renewable energy continues to decline, green hydrogen is expected to become more economically viable, enabling large-scale adoption across various sectors.

Another important trend is the integration of hydrogen energy systems with smart grids and energy storage solutions. Hydrogen can act as a long-term energy storage medium, helping to balance supply and demand in renewable energy systems. Excess energy generated during peak production periods can be converted into hydrogen and stored for later use, improving grid stability and reliability. Additionally, advancements in fuel cell technology are enhancing efficiency, durability, and cost-effectiveness, making hydrogen-powered systems more practical.

The expansion of hydrogen infrastructure and policy support is also shaping the future of this technology. Governments and industries worldwide are investing in hydrogen production, storage, and distribution networks to support a hydrogen-based economy. Emerging applications in sectors such as transportation, aviation, and heavy industries further highlight the versatility of hydrogen as an energy carrier. These developments indicate a strong transition toward a sustainable and hydrogen-driven energy landscape.

Conclusion

Hydrogen energy systems represent a transformative approach to achieving a sustainable and low-carbon energy future. By serving as a clean and versatile energy carrier, hydrogen has the potential to significantly reduce greenhouse gas emissions and dependence on fossil fuels. The integration of hydrogen with renewable energy sources further enhances its role in creating efficient and environmentally friendly energy systems.

While several challenges such as high production costs, storage complexities, and infrastructure limitations remain, continuous advancements in technology and increasing global investments are addressing these issues. The development of efficient production methods, improved storage solutions, and robust distribution networks is expected to accelerate the adoption of hydrogen energy systems in the coming years.

In conclusion, hydrogen energy holds immense potential as a key component of future energy systems. With ongoing research, policy support, and technological innovation, hydrogen is likely to play a central role in shaping a sustainable and energy-efficient global economy. A strong understanding of its challenges and future prospects is essential for realizing its full potential in modern energy applications.

References

1. J. O’M. Bockris and T. N. Veziroglu, “A solar–hydrogen energy system for sustainable development,” International Journal of Hydrogen Energy, vol. 32, no. 12, pp. 1605–1610, Aug. 2007.
2. M. Ball and M. Wietschel, “The future of hydrogen – opportunities and challenges,” International Journal of Hydrogen Energy, vol. 34, no. 2, pp. 615–627, Jan. 2009.
3. U. Eberle, M. Felderhoff, and F. Schüth, “Chemical and physical solutions for hydrogen storage,” Angewandte Chemie International Edition, vol. 48, no. 36, pp. 6608–6630, 2009.
4. A. Züttel, “Hydrogen storage methods,” Naturwissenschaften, vol. 91, no. 4, pp. 157–172, Apr. 2004.
5. S. Dunn, “Hydrogen futures: Toward a sustainable energy system,” International Journal of Hydrogen Energy, vol. 27, no. 3, pp. 235–264, Mar. 2002.
6. N. Armaroli and V. Balzani, “The future of energy supply: Challenges and opportunities,” Angewandte Chemie International Edition, vol. 46, no. 1–2, pp. 52–66, 2007.
7. I. Dincer and C. Acar, “Review and evaluation of hydrogen production methods for better sustainability,” International Journal of Hydrogen Energy, vol. 40, no. 34, pp. 11094–11111, Sep. 2015.
8. M. Momirlan and T. N. Veziroglu, “The properties of hydrogen as fuel tomorrow in sustainable energy system for a cleaner planet,” International Journal of Hydrogen Energy, vol. 30, no. 7, pp. 795–802, Jul. 2005.
9. A. Ursúa, L. M. Gandía, and P. Sanchis, “Hydrogen production from water electrolysis: Current status and future trends,” Proceedings of the IEEE, vol. 100, no. 2, pp. 410–426, Feb. 2012.
10. B. Sørensen, Hydrogen and Fuel Cells: Emerging Technologies and Applications, 2nd ed. London, U.K.: Elsevier, 2012.
11. R. O’Hayre, S. Cha, W. Colella, and F. B. Prinz, Fuel Cell Fundamentals, 2nd ed. Hoboken, NJ, USA: Wiley, 2009.
12. T. Smolinka et al., “Electrolysis for hydrogen production: Status and future,” Energy & Environmental Science, vol. 8, no. 6, pp. 1631–1644, 2015.
13. A. Godula-Jopek, Hydrogen Production by Electrolysis, Weinheim, Germany: Wiley-VCH, 2015.

14. M. Ni et al., “An overview of hydrogen production from biomass,” Progress in Energy and Combustion Science, vol. 32, no. 5–6, pp. 593–617, 2006.
15. L. Schlapbach and A. Züttel, “Hydrogen-storage materials for mobile applications,” Nature, vol. 414, pp. 353–358, Nov. 2001.

Frontiers in Chemical Science

ISBN: 978-93-49938-06-9| Year: 2026 | pp: 41 - 52 |

Hybrid Nanocomposite of Chitosan/Polyvinyl Alcohol and Green Synthesized Al2O3-SiO2 Nanoparticles for Food Packaging Application

[1]Dr. Arun K. Valvi

[1]Hemangi J. Gavit

[2]Dr. Sagar K. Patil

[3]Rohit S. Patil

[4]Dr. Nitin S. Sasane

[5]Dr. Gurumeet C. Wadhawa

[1]Rayat Shikshan Sanstha's Annasaheb Awate College, Manchar, Pune, Maharashtra, India.

[2]R&D Scientist, METTLER-TOLEDO India Private Limited, Mumbai, India.

[3]Department of Chemistry, Vasantrao Naik Mahavidyalaya, CIDCO, Chhatrapati Sambhajinagar, Maharashtra, India.

[4]Mahatma Phule Arts, Science and Commerce College, Panvel, Maharashtra, India

[5]Rayat Shikshan Sanstha's Veer Wajekar College. Punde, Navi Mumbai, Maharashtra, India.

Email: wadhava.gurumeet@gmail.com

Article DOI Link: https://zenodo.org/uploads/19637680

DOI: 10.5281/zenodo.19637680

Abstract

In the context of emerging global concerns with synthetic plastic packaging, alternative natural biodegradable packaging materials are gaining increasing attention for food packaging applications. In this study, Chitosan/Polyvinyl Alcohol nanocomposite hybrid films containing green synthesized Al2O3-SiO2 nanoparticles (NPs) were developed and microstructural properties were studied. Antimicrobial activity of the developed films was evaluated using both gram positive bacteria (Staphylococcus aureus) and gram negative (Escherichia coli). Green synthesis protocol was used for the precipitation of Al2O3-SiO2 NPs using extract of leaves of fimbristylis tetragona plant as capping agent. The as-synthesized crystalline Al2O3-SiO2 NPs average crystallite size was in the range of 39 nm. Reinforcement with Al2O3-SiO2 NPs in the hybrid films leads to improved thermal stability, elongation-at-break (EAB), and compactness properties. The developed films with 2% and 4% Al2O3-SiO2 NPs showed a smooth, compact, and heterogeneous surface morphology compared to the control (chitosan-gelatin hybrid) films. Disc discussion assays showed that the nanocomposite film had significant antimicrobial activity against E. coli. The developed hybrid nanocomposite films have the potential to be developed as a biodegradable alternative for post-harvest packaging of fresh fruits and vegetables.

Introduction

In these decades fast food or readymade food to eat or cook food is more popular. So, there is a need to increase the production of food. Al_2O_3-SiO_2 nanoparticles are gaining attention in food packaging applications due to their unique properties, which enhance the performance of packaging materials. These nanoparticles, when integrated into packaging films, significantly improve the material's barrier properties, mechanical strength, and thermal stability. The combination of aluminum oxide (Al_2O_3) and silicon dioxide (SiO_2) form a hybrid structure that offers excellent resistance to oxygen and moisture permeability, which is crucial in extending the shelf life of food products.

Chitosan is an important biopolymer with a wide range of applications, particularly in fields like food packaging, pharmaceuticals, agriculture, and biomedical sciences, due to its unique properties. Derived from chitin, which is found in the shells of crustaceans such as shrimp, crabs, and lobsters, chitosan is biodegradable, biocompatible, and non-toxic, making it a sustainable and environmentally friendly material.

One of the most significant aspects of chitosan is its antimicrobial activity. It has the ability to inhibit the growth of a wide range of bacteria, fungi, and other microorganisms, which is particularly useful in food packaging. When used in packaging materials, chitosan helps extend the shelf life of food by preventing microbial contamination and spoilage. This property is critical for preserving perishable items like fruits, vegetables, meat, and dairy products.

Chitosan also offers excellent film-forming capabilities. It can form thin, flexible films that are useful in various applications, particularly in edible coatings for food products and biodegradable packaging materials. These films act as barriers to gases like oxygen and moisture, which can spoil food by promoting oxidation and microbial growth. By incorporating chitosan into food packaging, the shelf life of products can be significantly extended while maintaining food quality.

Another important property of chitosan is its biodegradability. As environmental concerns regarding plastic waste continue to rise, chitosan presents an eco-friendly alternative to synthetic polymers in packaging. It decomposes naturally without leaving harmful residues, contributing to more sustainable packaging solutions.

Chitosan is also biocompatible, meaning it is safe for use in contact with living tissues and can be applied in areas such as wound healing and drug delivery systems. Its ability to bind with proteins and cells has been utilized in various biomedical and pharmaceutical applications, ranging from tissue engineering to targeted drug delivery.

Additionally, chitosan exhibits bioadhesive properties, which makes it an ideal candidate for applications where adherence to surfaces, such as biological tissues, is required. This feature is particularly valuable in developing controlled-release drug delivery systems or functional coatings for biomedical devices.

In agriculture, chitosan is used as a plant growth promoter and a natural pesticide. It stimulates plant growth and strengthens the plant’s immune system, helping crops resist diseases and environmental stresses.

Overall, chitosan's antimicrobial, biodegradable, biocompatible, and film-forming properties make it an invaluable material for a wide variety of applications, with its importance growing as industries seek more sustainable and eco-friendly alternatives to conventional materials.

In particular, Al_2O_3-SiO_2 nanoparticles create a more compact and organized structure within the packaging material, reducing the transmission of gases and water vapor that typically lead to spoilage. This barrier function is especially important for packaging fresh and processed foods, where maintaining an optimal internal environment can prevent oxidation and microbial growth. For instance, in meat or dairy packaging, the use of Al_2O_3-SiO_2 nanoparticles can help preserve freshness by limiting oxygen exposure and retaining moisture.

Additionally, these nanoparticles contribute to the mechanical strength of the packaging films, making them more resistant to tearing, punctures, or deformations. This enhances the durability of the packaging during handling and transport, ensuring that the food inside remains protected throughout its journey from producer to consumer. The inclusion of Al_2O_3-SiO_2 nanoparticles also improves the thermal stability of the packaging materials, allowing them to withstand higher temperatures without degrading, which is beneficial for packaging foods that undergo heat treatment or need to be stored in varying environmental conditions.

Moreover, Al_2O_3-SiO_2 nanoparticles can impart antimicrobial properties to the packaging, helping to inhibit the growth of harmful bacteria or fungi on the food surface. This is particularly important for perishable goods, as microbial contamination is one of the main factors that reduce food shelf life. The antimicrobial effect, combined with improved barrier and mechanical properties, makes packaging materials with Al_2O_3-SiO_2 nanoparticles highly effective for preserving food quality and safety.

In summary, the application of Al_2O_3-SiO_2 nanoparticles in food packaging enhances the protective functions of packaging films by providing superior barrier properties, mechanical robustness, and antimicrobial activity. These improvements contribute to the extended shelf life of food products while also ensuring the safety and integrity of the packaging material.

These can be prepared using a certain hygienic way. One of the important parameters is to protect the food against foodborne diseases. Nowadays, food borne diseases are widely increasing very rapidly [1-2]. Mostly foodborne diseases are increasing in various counties like the US around 76 million peoples a sufferer from this, 3,25,000 people can get affected and around 5000 die due to such diseases. It became necessary to develop antimicrobial and stable packing material. This packing material improves the quality of the food. They protect the food from microbes [3-4]. A hybrid nanocomposite of chitosan, polyvinyl alcohol (PVA), and green-synthesized Al_2O_3-SiO_2 nanoparticles represents an innovative approach to sustainable food packaging. Chitosan, a biodegradable and antimicrobial biopolymer, is blended with PVA, a synthetic polymer known for its excellent film-forming capabilities and mechanical strength. This combination improves the flexibility and durability of the material, making it suitable for food packaging applications.

Aluminum-silicon oxide (Al_2O_3-SiO_2) nanocomposites are advanced materials combining aluminum oxide (Al_2O_3) and silicon dioxide (SiO_2) nanoparticles. These nanocomposites offer enhanced mechanical strength, thermal stability, and barrier properties, making them valuable for a variety of applications.

Al_2O_3 provides hardness, wear resistance, and thermal conductivity, while SiO_2 adds toughness and electrical insulation. Together, they form a nanostructured material that is more durable, heat-resistant, and impermeable to gases and moisture.

In food packaging, Al_2O_3-SiO_2 nanocomposites improve the shelf life of products by preventing oxidation and moisture ingress. Their lightweight nature, combined with thermal and mechanical resilience, also makes them useful in aerospace, electronics, and catalysis.

Synthesis methods like sol-gel, co-precipitation, and hydrothermal techniques ensure uniform nanoparticle dispersion, which is critical to achieving the desired properties. These nanocomposites are also used in biomedical devices due to their biocompatibility and antimicrobial properties.

In summary, Al_2O_3-SiO_2 nanocomposites are versatile materials with applications in packaging, aerospace, electronics, catalysis, and healthcare, offering a balance of strength, heat resistance, and barrier efficiency.

Green synthesis of Al_2O_3-SiO_2 nanoparticles involves using biological methods such as plant extracts to reduce and stabilize the nanoparticles. This eco-friendly method avoids the use of harmful chemicals typically involved in conventional nanoparticle synthesis. The Al_2O_3-SiO_2 nanoparticles are introduced into the chitosan/PVA matrix to enhance the nanocomposite's mechanical, thermal, and barrier properties.

The resulting hybrid nanocomposite exhibits improved mechanical strength, elasticity, and gas barrier properties, making it more resistant to oxygen and moisture permeation. This is particularly important for extending the shelf life of food products. The antimicrobial properties of chitosan are further enhanced by the nanoparticles, providing an additional layer of protection against spoilage and microbial contamination.

Due to its biodegradable nature, this nanocomposite provides a sustainable alternative to conventional plastic packaging, reducing environmental waste while ensuring food safety and preservation. Its potential applications include packaging for perishable foods like fresh produce, meat, and dairy products, where both preservation and sustainability are critical concerns.

Most of the materials are inorganic which cannot react with the metal oxides or polymers or enzymes, the organic acids, enzymes and polymers and various metal oxides. The metal oxides have high temperatures [5-6]. Nanomaterials are newly developed materials, due to their good properties and features, they are used widely [7]. Such as nano-catalysts derived from plants are used for the synthesis of Benzimidazole derivatives [8-9]. In the last decades certain nanomaterials is used for food packing [10]. If a higher concentration of silver or other nanomaterial is present, they are not allowed for food packing. There are two types of nanomaterial packing was used such as packing in which the gases are trapped, in such case nanomaterials mixed with the polymer composites while in the second type the nanomaterial directly mixed with the food to get better antibacterial activity [11]. Metal nanoparticles with their potent antimicrobial properties are used for active packing. These are nanoparticles such as Ag, Au, Ti, Zn, Cu [12]. AgNPs and other nanoparticles can be hosted in different matrices and polymers with the agent as citrate and long chain polymeric alcohol. Among the many nanoparticles, the silver and aluminium oxide nanoparticles have a wide range of activity against fungi, viruses, yeasts and including bacteria [13]. These nanoparticles show very low volatility and good stability at high temperatures [14]. For such polymeric material, various strategies are used where the material was absorbed or directly incorporated in a synthetic process [15]. Furthermore, these nanoparticles have good properties. There is a certain risk associated with this due to the migration of the nanomaterial [16]. The food safety authority from Europe added the safety of the silver and aluminium nanoparticles [17]. According to the ESFA did provide the highest limit for the migration of the nanomaterial 0.05 mg/L in water and 0.05 mg/kg in food [18]. US FDA also gives certain rules for the packing of the food material, their metabolism and their mode of action [19]. Chitosan is a characteristic highly polysaccharide learned from the shells of shellfish by the deacetylation of chitin [20]. They have natural activity due to different functionality present. These may bring a surge of different proteins and microbial cells [21]. This chitosan is a nonlethal polymer with good antibacterial activity is a good choice for packing material [22]. Moreover, this study describes a promising method to enhance packaging material presently used in the food industry. Moreover, there is mammoth potential for this method in other food safeguarding applications. In the present work, plant assisted Aluminum oxide nanocomposite shows real antibacterial properties that can be used to augment the mechanical and block properties of chitosan aluminium oxide nanofilms. These can be easily fabricated. This may increase the capacity of the packing material. They are used in industrial food packing.

The plant used for the nanomaterial coating Fimbristylis tetragona R.Br., belongs to the family Cyperaceae (Sedge family) Fimbristylis tetragona R.Br., Prodr. Fl. Nov. Holl. 226. 1810; C. B. Clarke in Hook. F. Fl. Brit. India 6: 631. 1893; T. Cooke, Fl. Bombay 3: 393. 1958 (Repr. ed.). Perennial with the short rhizome. Phenology- Flowering: August–September; Fruiting: September–December. Voucher specimen: ANC 1727.

Collection localities: Abasaheb Marathe College, Vikhare Gothane, Rajapur tehsil of Ratnagiri District (Maharashtra). Distribution: Fimbristylis tetragona is distributed in tropical Asia and Australia. In India, it occurs in Bihar, Gujarat, Goa, Karnataka, Kerala, Maharashtra, Meghalaya, Orissa, Rajasthan, Tamil Nadu, Uttar Pradesh, Madhya Pradesh, Andhra Pradesh and West Bengal. Illustrations: K. M. Matthew, Further Illus. Fl. Tamilnadu Carnatic 4: t. 675.1988; C. B. Clarke, Illus. Cyp. t. 40, f. 1-4. 1909 [23-24].

Experimental Material and Methods

Materials

Chitosan is a natural polymer having an average molecular weight 92,700 g mol−1, and it can be deacylated at 82.5 purchased from S. D. fine limited. Polyvinyl alcohol and acetic acid, ammonium hydroxide, aluminium sulfate and SiO2 Powder were also purchased from S. D. Fine limited. Leaves obtained from the plant were dried in shade for 3 weeks. Then dried in the oven for 300C till constant weight was obtained. These are grinding into fine powder; the powder is dried at 400C for 6h or till constant weight was obtained and then stored in an air tight container.

Preparation of Aluminium-Si oxide Nanocomposites

The aluminum nanoparticles were prepared by the coprecipitation method aluminium sulfate, 0.1M was taken in distilled water. 0.2M of NaOH solution was added with stirring over the sonication. We have added water extract from the leaves of the plant as a capping agent, 1 g of the SiO2 NPs. The obtained creamy solution was kept for 6h for settling down and upper solution remove easily. The precipitated washed several times with water then dried at 900C for 12h till constant weight was obtained. The precipitated heated at the 500 0C for 3h to obtain alumina silica nanocomposites. Chitosan was placed in 5 mL of the acetic acid (2%) at temperature to get a homogenous solution. The synthesis of the aqueous PVA solution at 800C by mixing PVA polymer in distilled water. The PVA/CS (70:30 wt/wt) was blended and the solution was stirred. Bio-nanocomposites Al2O3-SiO2 loading at 0.5, 1, 3, 5 % w/v created through the Al2O3-SiO2 suspension of 1mg/mL in water to the PVA/CS and sonicated for 4 h. The homogeneous suspension of PVA/ Al2O3-SiO2 was taken in the Teflon plate and kept for 85 h at room temperature to get the film. The film of PVA/CS/Al2O3-SiO2 was taken out of the mould. Then it was characterized and used for packing material. All measurements were carried out by the standard protocol.

Results and discussion

Infrared Spectral Analysis

The IR Spectra Fig.1 was recorded on the Shimadzu IR Infinity from 400-4000cm-1 on the IR spectra. Si-O-Si bond occurs at 1196 cm-1, Al-O-Al bond occurs at 1116 cm-1, Si-O-Al bond occurs at 596 cm-1, Al-O bond occurs at 596 cm-1 and Al-O bond occurs at 596 cm-1.

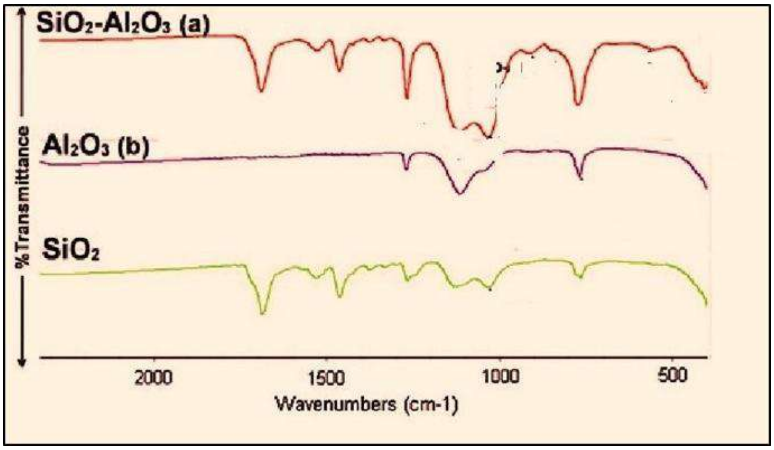


Fig.1. FTIR Spectra of SiO2, Al2O3 and SiO2-Al2O3.

X-ray Diffraction (XRD)

X-ray diffraction (XRD) is an analytical technique used to study the crystallographic structure of materials. When X-rays are directed at a crystalline sample, they interact with the crystal lattice and are diffracted in specific directions based on the atomic arrangement. By measuring the angles and intensities of the diffracted beams, the crystal structure, phase composition, and grain size of the material can be determined. XRD is widely used in material science to identify compounds, analyze crystalline phases, and assess the purity and structural properties of solids. The x-ray diffraction Fig.2 was measured using an X-ray Philips diffract meter fixed with radiation. Fixed with radiation of Cu lamp Kα

(45kV, 40mA, with λ=0.15418nm). In 2 theta degree of the scanning. The Al2O3-SiO2 nanocomposites were studied using the XRD. The XRD pattern of synthesized Al2O3-SiO2 nanocomposites is carried at 2 theta values for Al2O3 32.00, 34.89, 36.67, 47.87, 56.78, 62.90, 67.90, 70. The peak of the planes agree with (100), (002), (101), (102), (110), (103), (112) and (201) 2 theta values for SiO2 22.00, 39.00, 45.00, 77.67, 76.67 and planes occur at (100), (110), (111), (220) and (221).

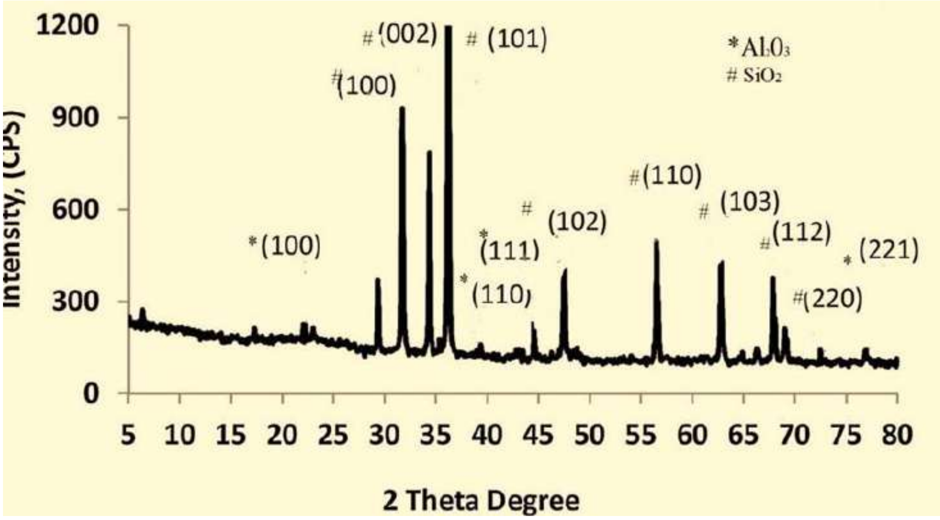


Fig.2. X-ray diffraction (XRD)

Barrier Properties

The barrier properties Table2 can be measured using the GBI W303(B) and the water permeability analyzer water vapours transmission rate was measured using the CUP procedures. The amount of the water vapours coming out of the film was tested for the test film. The water vapour permeability as well as the gas transmission rate of the prepared nano biocomposites.

Table1: Barrier properties of various synthesized biopolymers.

Samples	**Al2O3-SiO2**	**OTR, g/(cc/m^2.day)**	**WVTR, g/(m^2.day)**
PVA/CS	0.0 Al2O3-SiO2	150	900
PVA/CS	0.5% Al2O3-SiO2	140	970
PVA/CS	1% Al2O3-SiO2	90	1010
PVA/CS	3% Al2O3-SiO2	70	1050
PVA/CS	5% ZnAl2O3-SiO2	50	1110

Scanning Electron Microscopy (SEM) and EDX Measurement

SEM Fig.3 was recorded with SEM, JSM6360. This was used to study the morphology of the filmed dispersive energy spectrometer (EDX) to which microscope carried at 10-15 kv as accelerating voltage. This was carried out using the low deposition rate.

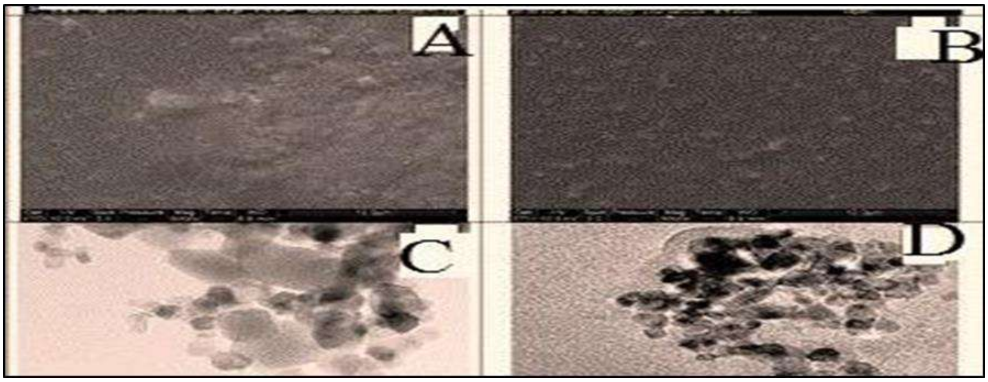


Fig 3. SEM images of the prepared PVA/CS blend, a) PVA/CS Al2O3SiO3 bio-nanocomposites, b) at concentration 0.5%, c) at concentration 1%, d) at concentration 5%.

The morphological analysis of the various Bio-nanocomposites film was evaluated using the scanning electron microscope. This was also carried out for 0.5, 1.0 and 5% indicate that the good particle size of the material.

Antibacterial Activity

Antimicrobial Activity Table2 of the polyvinylalcohol/chitosan (PVA/CS) was carried out with the different concentration Al2O3-SiO2 nanoparticles. As (0.5, 1,3 and5%) was studied using the zone of inhibition method. Certain gram-positive and Gram-negative bacteria were used. For this Specific protocol was used.

Table 2: Concentrations of Al2O3-SiO2 against Common Bacteria.

Sample	**Sta9**	**Escherichia coli**
PVA/CS	0	0
0.5% Al2O3-SiO2	23	28
1%Al2O3-SiO2	25	31
3%Al2O3-SiO2	32	37
5%ZnAl2O3-SiO2	39	41

The result of the antibacterial activity shown was better and had the good activity against the different compositions of the Al2O3-SiO2 nanocomposites.

Table 3: Mechanical Properties of the synthesized biopolymers.

Samples	**% Al2O3-SiO2**	**Tensile strength Pa**	**Elongation (%)**
PVA/CS	0.00	2.71x107	60.00
CS	0.00	1.58x107	95.00
Al2O3-SiO2	0.5%	7.68x107	78.00
Al2O3-SiO2	1%	6.61x107	110.00

Al2O3-SiO2	3%	5.71x107	120.00
Al2O3-SiO2	5%	4.81x107	130.00

The results of the mechanical properties in Table 3 indicate that various Nanocomposites have good tensile strength and the% of elongation. We have synthesized the biopolymer using the nanocomposite of the Al2O3-SiO2. During the synthesis of this nanocomposite, we used the leaves of the Fimbristylis tetragona plant. The various natural products present in leaf powder act as a capping agent for this nanocomposite instead of the chemical regent. The formation of this nanocomposite has been proved using IR spectroscopy. The nature of the nanocomposite is proved by the XRD. The morphology is given by the SEM and EDX analysis. The synthesized biocomposites are converted to biopolymer using various natural polymeric material. The synthesized biopolymer contains various % of the nanocomposites and shows good antimicrobial activity. It shows all properties required for the biopolymer.

Conclusion

The study demonstrates that various bionanocomposite films of PVA/CS/Al_2O_3-SiO_2 exhibit satisfactory tensile strength, along with excellent gas and water vapor barrier properties. These films, synthesized using chitosan and polyvinyl alcohol with varying percentages of Al_2O_3-SiO_2, show strong antibacterial activity against common bacterial strains. The findings suggest that these nanocomposites provide an improved material for food packaging. A green synthesis approach was employed, using plant leaves as a natural coating material for the production of nanomaterials. This eco-friendly method highlights the potential of sustainable, green chemistry in developing high-performance packaging solutions.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The authors are thankful to the Rayat Shikshan Sanstha, Satara for providing research facilities.

References

1. P. Kaewklin, U. Siripatrawan, A. Suwanagul & Y. S. Lee, "Active packaging from chitosan titaniumdioxide nancomposite film for prolonging storage life of tomato fruit". International Journal of Biological Macromolecules, 112, (2018) 523–529.
2. J. K. Morris, "To How safe is our food?" Emerg. Infect. Dis. 17, (2011) 26-128.

3. L. Vermeiren, F. Devlieghere, J. Debevere, "Effectiveness of some recent antimicrobial packaging concepts", Food Addit. Contam. 19, (2002) 163-171.
4. B. Malhotra, A. Keshwani, H. Kharkwal, "Antimicrobial food packaging: potential and pitfalls," Frontiers Miocrobiol. 6, (2015) 1-9.
5. A. M. Metak, "Effects of Nanocomposites based nano-silver and nano-titaniumdioxide on food packaging materials", Int. J. Appl. Sci. Technol. 5, (2015) 26-40.
6. A. M. Metak, T. T. Ajaal, "Investigation on polymer-based nano-silver as food packaging materials," Int. J. of Biological, Food, Veterinary and Agricultural Engineering, 7, (2013) 772-777.
7. M. Carbone, G. Sabbatella, S. Antonaroli, H. Remita, V. Orlando, S. Biagioni, A. Nucara, "Exogenous control over intracellular acidification: Enhancement via proton caged compounds coupled to gold nanoparticles," Biochim. Biophys. Acta, gen. Sub., 1850, (2015) 2304-2307.
8. G. C. Wadhawa, A. K. Valvi, R. D. Mohite, D. D. Patil, B. Patil, H. J. Gavit, An Organo-Heterogeneous catalyst for synthesis of benzimidazole derivatives using nanoparticles synthesized from Plant extract and supported on Montmorillonite K10, Materials Today: Proceedings, Volume 58, Part 2, (2022) Pages 764-768.
9. A. K. Valvi, S. S. Nayak, V. S. Shivankar, G. C. Wadhawa, Nano catalyst derived from plant Polyzygus Tuberosus: A suitable for efficient and green synthesis of benzimidazole derivatives, Materials Today: Proceedings, Volume 50, Part 5, 2022, Pages 1522-1526.
10. N. Bumbudsanpharoke, S. Ko, "Nano-food packaging: an overview of market, migration research and safety regulations," J of Food Science, 80, (2015) R910-R923.
11. T. V. Duncan, "Applications of nanotechnology in food packaging and food safety: barrier materials, antimicrobials and sensors," J of Colloid and Interface Science, 363, (2011) 1-24.
12. R. D. Toker, N. Kayaman-Apohan, M. V. Kahraman, "UV-curable nano-silver containing polyurethane based organic-inorganic hybrid coatings," Prog. Org. Coat. 76, (2013) 1243-1250.
13. M. Rai, A. Yadav, A. Gade, "Silver nanoparticles as a new generation of antimicrobials.," Biotechnol. Adv. 27, (2009) 76-83.
14. A. M. Youssef, M. S. Abdel-Aziz, "Preparation of polystyrene nanocomposites based on silver nanoparticles using marine bacterium for packaging," Polymer-Plastics Technol. Eng. 52, (2013) 607-613.
15. A. Martinez-Abad, J. M. Lagaron, M. J. Ocio, Development and characterization of silver based antimicrobial ethylene-vinylalcohol copolymer (EVOH) films for food-packaging applications, J. Agric. Food Chem. 60 (21), (2012) 5350-5359.

16. M. Cushen, J. Kerry, M. Morris, M. Cruz-Romero, Cummins, "Nanotechnologies in the food industry – recent developments, risks and regulation review article," Trends in Food Sci. & Technol. 24, (2012) 1-60.
17. Shenir (Scientific Committee on Emerging and Newly Identified Health Risks) 2014, http://ec.europa.eu/health/scientific_committees/policy/index_en.htm
18. [EFSA] European Food Safety Authority. 2011. Guidance on the risk assessment of the application of nanoscience and nanotechnology in the food and feed chain. EFSA J 9(5), 2140.
19. [USFDA] United States Food and Drug Administration. 2014. Guidance for industry: assessing the effects of significant manufacturing process changes, including emerging technologies on the safety and regulatory status of food ingredients and food contact substances, including food ingredients that are color additives. Available from: http://www.fda.gov/Food/GuidanceRegulation/GuidanceDocumentsRegulatoryInformation/IngredientsAdditivesGRASPackaging/ucm300661.htm. Accessed 2014 November 05.
20. E. M. D. A. Braz, S. C. Cavalcante Costa E Silva, D. A. D. Silva, F. A. D. A. Carvalho, H. M. Barreto, L. D. S. S. Júnior, etal. Modified chitosan-based bioactive material for antimicrobial application: Synthesis and characterization. International Journal of Biological Macromolecules, 117, (2018) 640–647. https://doi.org/10.1016/j. ijbiomac.2018.05.205
21. H. Moustafa, A. M. Youssef, N. A. Darwish, & A. I. Abou-Kandil, "Eco-friendly polymer composites for green packaging: Future vision and challenges." Composites Part B Engineering, 172, (2019), 16-25.
22. O. M. Sharaf, M. S. Al-Gamal, G. A. Ibrahim, N. M. Dabiza, S. S. Salem & M. F. El- ssayad, "Evaluation and characterization of some protective culture metabolites in free and nano- chitosan-loaded forms against common contaminants of Egyptian cheese," Carbohydrate Polymers, 223, (2019) Article, 115094.
23. T. Cooke, (1905): The Flora of the Presidency of Bombay. Vol.2, Taylor & Francis, London. Pp. 879. (Repr.ed.3: 393. 1958).
24. J. D. Hooker, (1893): Flora of British India Vol. 6, L. Reeve & Co, London. p. 631.

Frontiers in Chemical Science

ISBN: 978-93-49938-06-9| Year: 2026 | pp: 53 – 69 |

Hydrogen Production Technologies

[1]R. Deivanayaki

[1]M. Aswini

[1]S. Immanuel Prabaharan

[2]Dr. S. Muthurajan

[3]Dr. Arul Kulandaivel

[1]Research Scholar - EEE Dept., AMET University - Kanathur, Chennai - 603112.

[2]Assistant Professor - Marine Dept., AMET University - Kanathur, Chennai - 603112.

[3]Director and Professor – Robotics and Automation Engineering, Dhaanish Ahmed Institute of Technology, Coimbatore – 641105

Email: deivanayakiphd@ametuniv.ac.in

Article DOI Link: https://zenodo.org/uploads/19637796

DOI: 10.5281/zenodo.19637796

Abstract

Hydrogen has emerged as a pivotal clean energy carrier in the global transition toward decarbonized energy systems, offering high gravimetric energy density and versatility across sectors. This chapter examines the fundamental technologies for hydrogen production from conventional methods such as steam methane reforming and coal gasification to advanced pathways including water electrolysis, photocatalytic splitting, and biological techniques and evaluates their potential within sustainable energy frameworks. With the increasing integration of renewable energy sources, electrolytic hydrogen production, particularly via alkaline, proton exchange membrane (PEM), and solid oxide electrolysis, has gained prominence due to its high purity output and low emissions when powered by renewables. The development of efficient electrolyzers is critical for enabling sector coupling between power systems and hydrogen infrastructure, as reviewed in recent literature.

The chapter further explores the intersection of hydrogen technologies with electric vehicle (EV) powertrains and Battery Management Systems (BMS). Fuel cell electric vehicles (FCEVs) leverage hydrogen to generate electricity in real time,

complementing battery electric vehicles (BEVs) and addressing limitations in range and refuelling times. Integration of hydrogen storage, fuel cells, and EV BMS necessitates advanced electrical and electronics engineering (EEE) solutions including power conditioning, real time monitoring, and dynamic control to optimize performance, safety, and energy management. Case studies in hydrogen vehicular applications illustrate the practical challenges and opportunities of these integrated systems. Despite significant technological progress, barriers related to cost, scalability, infrastructure, and regulatory frameworks remain. This chapter synthesizes current advancements and outlines future research directions emphasizing hybrid renewable hydrogen systems, smart grid interaction, and BMS innovations highlighting hydrogen's potential to enhance sustainability in the EV and broader EEE ecosystem.

Introduction

1. Overview of Hydrogen as a Clean Energy Carrier

Hydrogen is increasingly recognized as a versatile and sustainable energy carrier with the potential to transform the global energy landscape. Unlike conventional fossil fuels, hydrogen combustion produces water as the primary by product, making it an environmentally benign alternative for power generation, transportation, and industrial applications. Its high gravimetric energy density allows for efficient storage and transportation, making hydrogen a promising candidate for bridging the intermittency of renewable energy sources. Advances in production, storage, and distribution technologies have positioned hydrogen as a key enabler of a low-carbon energy economy, with applications ranging from grid-scale energy storage to fuel cell-powered electric vehicles (FCEVs).

2. Importance of Hydrogen in De-carbonization and Energy Transition

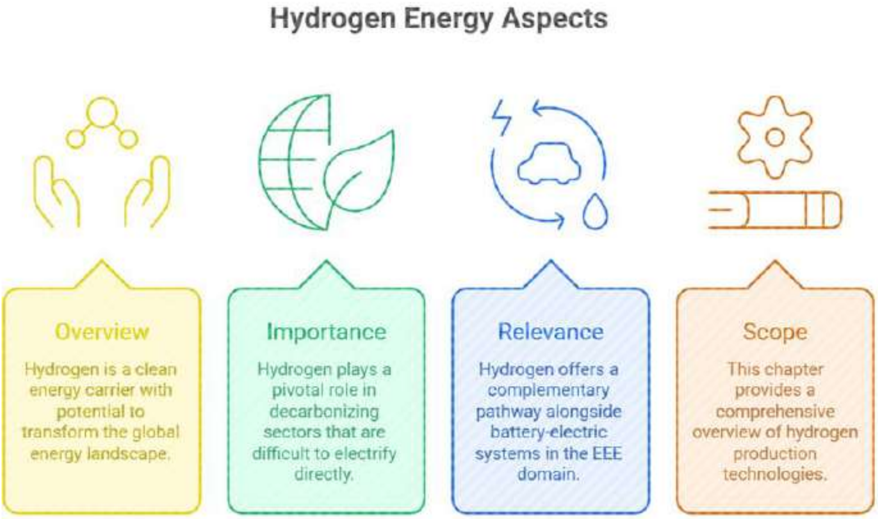
The global push towards net-zero carbon emissions has accelerated research into hydrogen as a clean energy vector. Hydrogen plays a pivotal role in decarbonizing sectors that are difficult to electrify directly, such as heavy industry, shipping, and aviation. When produced via low-carbon methods such as water electrolysis using renewable electricity, hydrogen can significantly reduce greenhouse gas emissions. Moreover, its integration into energy systems allows for the storage of surplus renewable electricity, enabling grid stability and load balancing. The versatility of hydrogen, coupled with its compatibility with existing infrastructure through blending or direct usage, underscores its importance in the ongoing transition towards sustainable energy.

3. Relevance to EVs, Renewable Integration, and the EEE Field

In the context of electric vehicles (EVs) and the broader electrical and electronics engineering (EEE) domain, hydrogen offers a complementary pathway alongside battery-electric systems. Fuel cell electric vehicles (FCEVs) leverage hydrogen to generate electricity on-demand, providing longer driving ranges and faster refueling times compared to conventional batteries. This convergence necessitates sophisticated electrical management, including integration with battery management systems (BMS) to ensure efficient energy flow, safety, and performance optimization. Additionally, hydrogen-based systems can interact with renewable energy sources, acting as an energy buffer, while EEE technologies play a critical role in power conversion, monitoring, and control, ensuring reliable and efficient hydrogen utilization.

4. Scope of the Chapter

This chapter provides a comprehensive overview of hydrogen production technologies with an emphasis on their relevance to the EV sector and electrical engineering applications. It explores conventional and emerging production methods, their operational principles, efficiency considerations, and integration with renewable energy systems. Furthermore, it examines the intersection of hydrogen storage, fuel cells, and battery management systems, highlighting technological challenges and opportunities. By bridging chemical science with EEE principles, the chapter aims to present a holistic perspective on how hydrogen can contribute to sustainable transportation and energy systems.



Overview
Hydrogen is a clean energy carrier with potential to transform the global energy landscape.

Importance
Hydrogen plays a pivotal role in decarbonizing sectors that are difficult to electrify directly.

Relevance
Hydrogen offers a complementary pathway alongside battery-electric systems in the EEE domain.

Scope
This chapter provides a comprehensive overview of hydrogen production technologies.

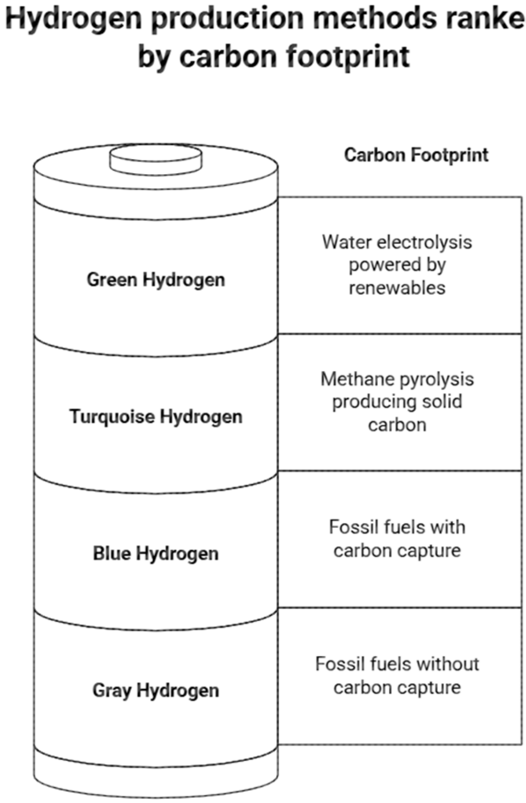
Fundamentals of Hydrogen Production

1. Basic Chemistry of Hydrogen Generation

Hydrogen can be generated through several chemical and electrochemical processes, each with unique mechanisms, energy requirements, and environmental impacts. Water splitting is a fundamental route, where water molecules are decomposed into hydrogen and oxygen through thermal, photochemical, or electrochemical methods. In electrolysis, an external electric current drives the separation of water into hydrogen and oxygen, providing a clean pathway when powered by renewable electricity. Hydrocarbon reforming, including steam methane reforming (SMR) and partial oxidation, involves extracting hydrogen from fossil fuels by breaking chemical bonds with high-temperature reactions, often generating CO_2 as a byproduct. These production pathways form the foundation of hydrogen generation, and understanding their chemistry is crucial for integrating hydrogen systems into renewable and electric vehicle infrastructures.

2. Hydrogen Classification: Gray, Blue, Green, Turquoise

Hydrogen is commonly classified based on its production method and associated carbon footprint. Gray hydrogen is produced from fossil fuels such as natural gas without carbon capture, resulting in significant CO_2 emissions. Blue hydrogen follows the same process but incorporates carbon capture and storage (CCS) technologies to reduce emissions. Green hydrogen is generated via water electrolysis powered entirely by renewable energy sources, offering a near-zero-emission solution. Turquoise hydrogen involves methane pyrolysis, producing solid carbon instead of CO_2, presenting a promising low-emission alternative. This classification is essential for evaluating the environmental impact of hydrogen use in EVs and energy systems, guiding engineers and researchers toward sustainable options.



3. Energy Efficiency Considerations

Energy efficiency is a critical factor in hydrogen production, influencing both economic viability and environmental impact. Electrolysis efficiency depends on the type of electrolyzer, operating conditions, and power source, with modern PEM and solid oxide electrolyzers achieving efficiencies of 60–80%. Hydrocarbon-based methods, while mature and cost-effective, incur energy losses in high-temperature reactions and CO_2 management. Integrating hydrogen production with renewable energy sources, smart grid operations, and EV charging infrastructure requires careful assessment of energy conversion, storage losses, and system-level efficiency. Optimization of these factors ensures that hydrogen remains a competitive and sustainable energy carrier.

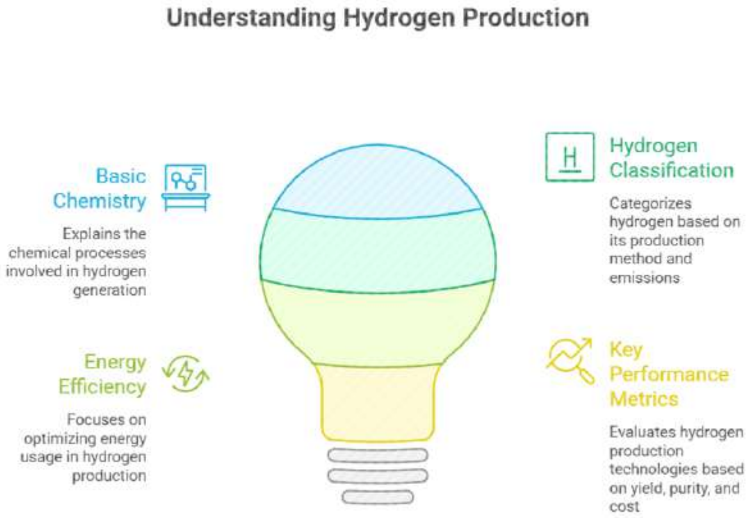
4. Key Performance Metrics (Yield, Purity, Cost)

The evaluation of hydrogen production technologies relies on several performance metrics. Yield refers to the amount of hydrogen produced per unit of feedstock or electricity input, influencing scalability and operational efficiency.

Purity is critical for downstream applications, particularly in fuel cells, where impurities can degrade performance and reduce lifespan.

Cost encompasses capital investment, operational expenses, and energy costs, determining the commercial viability of hydrogen production methods.

For EV and EEE applications, high purity and reliable yield are essential for safe and efficient integration with fuel cells, batteries, and power electronics, highlighting the need for robust and optimized hydrogen generation technologies.



Understanding Hydrogen Production

Conventional Hydrogen Production Methods

1. Steam Methane Reforming (SMR)

- **Process Description**

Steam Methane Reforming (SMR) is the most widely used method for industrial hydrogen production. In SMR, methane (CH_4), typically sourced from natural gas, reacts with steam at high temperatures (700–1,100 °C) in the presence of a nickel-based catalyst to produce hydrogen (H_2) and carbon monoxide (CO). This is followed by a water-gas shift reaction, where CO reacts with water to generate additional H_2 and CO_2. The overall process efficiently converts hydrocarbons into hydrogen, making SMR economically attractive and scalable.

- **Advantages, Limitations, Emissions**

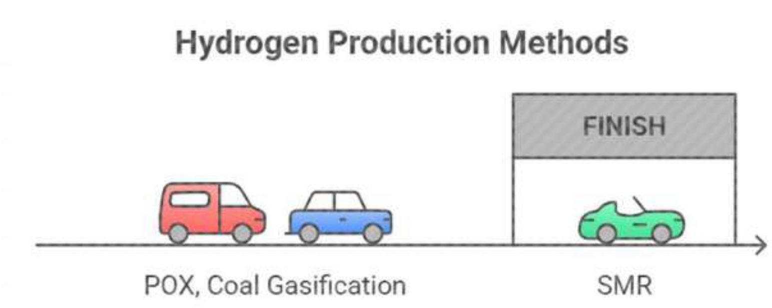
SMR's primary advantage lies in its high hydrogen yield and established industrial infrastructure. It is cost-effective compared to most other production methods and can be operated continuously at large scale. However, SMR has significant limitations from an environmental perspective. The process emits substantial CO_2 unless paired with carbon capture and storage (CCS) technology. Additionally, it relies on fossil fuel feedstocks, which may not align with decarbonization goals. In the context of EV and fuel cell applications, SMR-produced hydrogen can serve as a supply for refueling stations, but integrating it sustainably with renewable energy systems and battery/fuel cell management requires careful consideration of emissions and system efficiency.

2. Partial Oxidation of Hydrocarbons

Partial oxidation (POX) is an alternative method in which hydrocarbons such as natural gas, diesel, or heavy oils are partially combusted with limited oxygen, producing a mixture of hydrogen and carbon monoxide (syngas). POX is faster than SMR and operates at higher temperatures (900–1,500 °C), making it suitable for feedstocks with higher carbon content. While the process can produce hydrogen without the need for external steam, it also generates CO_2 and requires downstream treatment to remove impurities. From an EEE perspective, hydrogen from POX can be integrated with fuel cell systems for EVs, but its fluctuating composition may necessitate advanced power electronics and BMS algorithms to manage variable energy quality and storage.

3. Coal Gasification

Coal gasification involves the high-temperature reaction of coal with oxygen and steam to produce syngas, which is further processed to extract hydrogen. This method allows hydrogen production from abundant coal reserves, but it is associated with high CO_2 emissions and complex waste management. Despite environmental concerns, coal gasification remains relevant in regions with limited natural gas or renewable resources. For EV applications, hydrogen from coal gasification can feed fuel cells, but system designers must address the impact of impurities on fuel cell longevity and implement robust BMS and power conditioning systems to maintain efficiency and safety.



Electrolytic Hydrogen Production

1. Water Electrolysis

Water electrolysis is a clean and versatile method for producing hydrogen by splitting water into hydrogen and oxygen using electrical energy. Unlike hydrocarbon-based methods, electrolysis can operate entirely carbon-free when powered by renewable energy sources, making it highly relevant for sustainable energy systems and EV applications. Electrolysis can be performed using various technologies, each with distinct operational characteristics:

- **Alkaline Electrolysis**

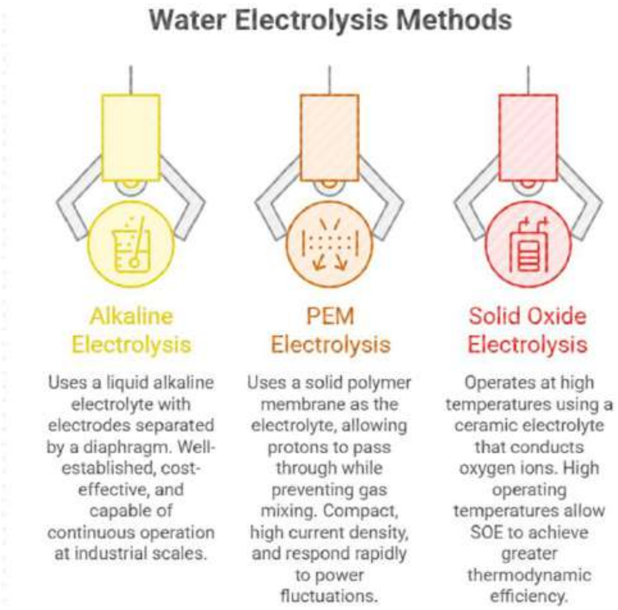
Alkaline electrolysis uses a liquid alkaline electrolyte, typically potassium hydroxide (KOH) or sodium hydroxide (NaOH), with electrodes separated by a diaphragm. This method is well-established, cost-effective, and capable of continuous operation at industrial scales. However, alkaline electrolyzers have slower response times to fluctuating power input, which can limit their integration with variable renewable energy sources.

- **Proton Exchange Membrane (PEM) Electrolysis**

PEM electrolysis uses a solid polymer membrane as the electrolyte, allowing protons to pass through while preventing gas mixing. PEM systems are compact, have high current density, and respond rapidly to power fluctuations, making them highly compatible with intermittent renewable energy sources and dynamic load management. Their fast response and high purity output make them particularly suitable for EV hydrogen fueling stations where rapid hydrogen supply is essential.

- **Solid Oxide Electrolysis (SOE)**

SOE operates at high temperatures (typically 700–1,000 °C) using a ceramic electrolyte that conducts oxygen ions. High operating temperatures allow SOE to achieve greater thermodynamic efficiency by utilizing both electrical and thermal energy. SOE is attractive for large-scale hydrogen production, particularly when integrated with high-temperature industrial waste heat, but it presents challenges in material durability and startup times.



Water Electrolysis Methods

Alkaline Electrolysis

Uses a liquid alkaline electrolyte with electrodes separated by a diaphragm. Well-established, cost-effective, and capable of continuous operation at industrial scales.

PEM Electrolysis

Uses a solid polymer membrane as the electrolyte, allowing protons to pass through while preventing gas mixing. Compact, high current density, and respond rapidly to power fluctuations.

Solid Oxide Electrolysis

Operates at high temperatures using a ceramic electrolyte that conducts oxygen ions. High operating temperatures allow SOE to achieve greater thermodynamic efficiency.

2. Integration with Renewable Energy Sources

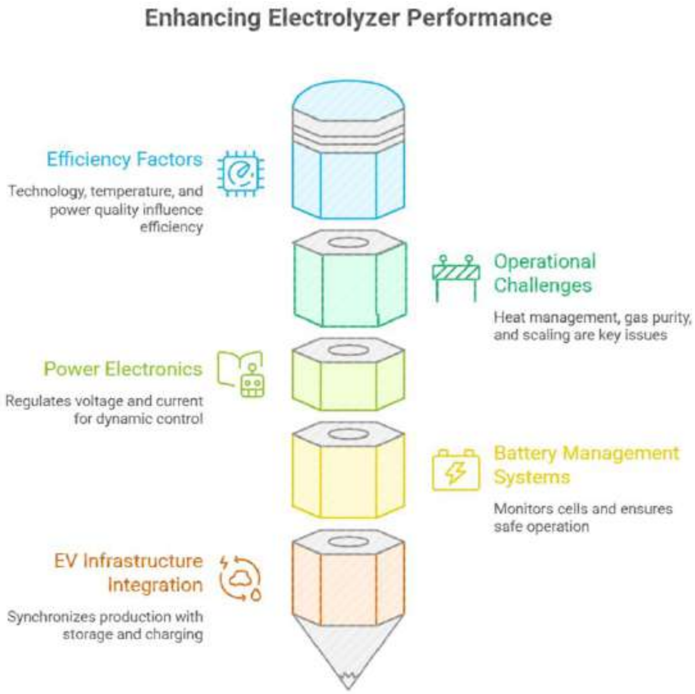
Electrolytic hydrogen production is ideally suited for coupling with renewable energy, such as solar and wind. Surplus electricity from these intermittent sources can be stored in the form of hydrogen, providing a form of energy buffering and enabling grid balancing. In EV systems, this approach allows hydrogen fuel cell infrastructure to be supplied sustainably, minimizing dependence on fossil fuels. Integration requires sophisticated energy management strategies to match electrolyzer operation with fluctuating power availability while maintaining efficiency and system stability.

3. Efficiency and Operational Challenges

Electrolyzer efficiency depends on technology type, operating temperature, and input power quality. Alkaline and PEM electrolyzers typically achieve efficiencies between 60–80%, while high-temperature SOE can reach 85% under optimal conditions. Challenges include managing heat, gas purity, scaling the systems for industrial hydrogen supply, and minimizing degradation over time. For EV applications, maintaining consistent hydrogen purity is critical to avoid fuel cell performance loss, emphasizing the importance of monitoring and control systems.

4. Role of Power Electronics and BMS in Electrolyzers

Electrical and electronics engineering plays a central role in modern electrolyzers. Power electronics regulate voltage and current, manage AC/DC conversion, and allow dynamic control for load-following with renewable sources. Battery management systems (BMS) and advanced control units are used to monitor electrolyzer cells, track voltage, temperature, and hydrogen output, and ensure safe operation. In EV-related hydrogen infrastructure, these systems are critical for synchronizing hydrogen production with storage, fuel cell operation, and charging stations, optimizing both energy efficiency and reliability.



Emerging and Advanced Hydrogen Production Technologies

1. Photocatalytic and Photo-electrochemical Water Splitting

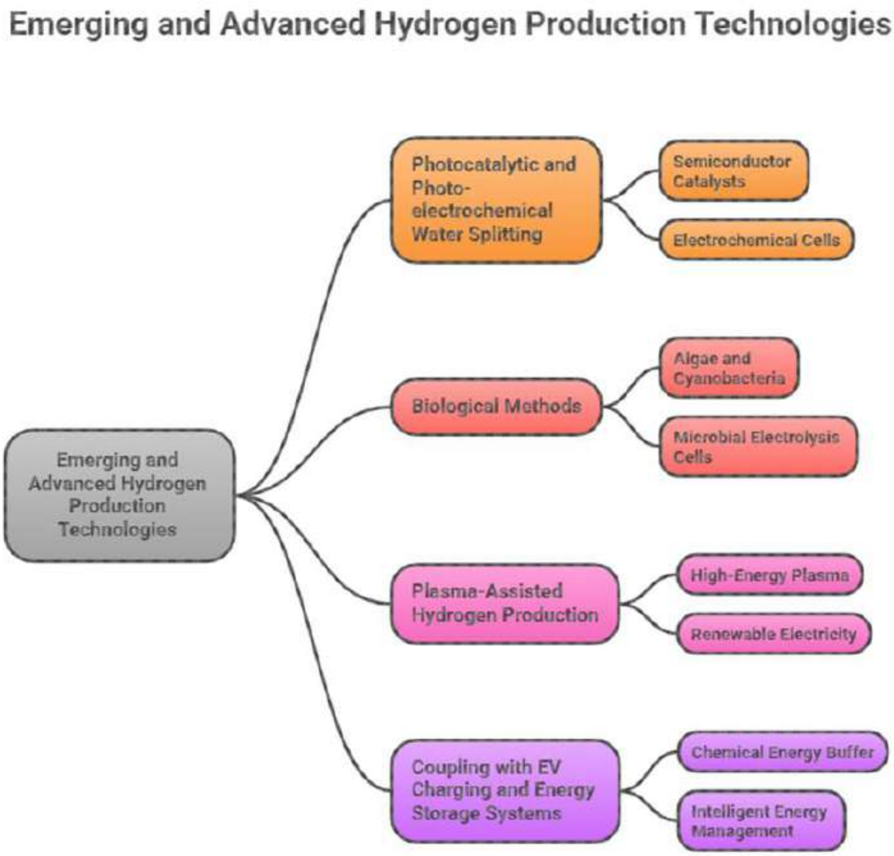
Photocatalytic and photo-electrochemical (PEC) water splitting represents promising routes for direct solar-to-hydrogen conversion. In photocatalytic water splitting, semiconductor catalysts absorb sunlight and drive water decomposition at the surface, producing hydrogen and oxygen without external electricity. PEC systems integrate light-absorbing electrodes with electrochemical cells, where photons generate electron-hole pairs to facilitate hydrogen production. These methods offer the potential for highly sustainable hydrogen generation, bypassing the need for fossil fuels entirely. However, challenges such as low solar-to-hydrogen efficiency, material stability, and scalability remain. From an EV and EEE perspective, PEC and photocatalytic systems could eventually supply distributed hydrogen for local fuel cell charging stations, integrated with smart power electronics and energy management systems to ensure reliable hydrogen output.

2. Biological Methods: Algae, Bacteria, Microbial Electrolysis

Biological hydrogen production leverages living organisms to convert biomass or water into hydrogen. Algae and cyanobacteria can produce hydrogen via photosynthetic pathways under specific conditions, while microbial electrolysis cells (MECs) use bacteria to catalyze water splitting in bioelectrochemical systems. These methods are inherently sustainable and can utilize organic waste streams, offering a dual benefit of energy generation and waste treatment. However, low production rates, sensitivity to environmental conditions, and complexity of scaling up remain major hurdles. Integrating these biohydrogen systems with EV infrastructure would require hybrid energy systems and advanced BMS to manage intermittent hydrogen availability and ensure consistent fuel cell performance.

3. Plasma-Assisted Hydrogen Production

Plasma-assisted hydrogen production utilizes high-energy plasma to dissociate water or hydrocarbons into hydrogen and other byproducts. The technique allows for fast reactions at relatively low bulk temperatures and offers potential for high-purity hydrogen production. Plasma methods can be powered by renewable electricity, providing a flexible, modular, and potentially carbon-neutral solution. In EV applications, plasma-generated hydrogen could be directly linked to refueling or storage systems, with power electronics managing the energy input and BMS ensuring safe operation of hydrogen storage and fuel cells.



4. Coupling with EV Charging and Energy Storage Systems

Emerging hydrogen production technologies are increasingly designed to interface with EV charging and energy storage infrastructure. Hydrogen can act as a chemical energy buffer, storing excess renewable energy during periods of low grid demand and supplying fuel to FCEVs when needed. Hybrid systems combining batteries and hydrogen fuel cells require intelligent energy management, where BMS and power electronics coordinate charging, discharging, and hydrogen generation to optimize efficiency and extend system lifetime. Advanced control algorithms can balance the intermittent supply of renewables, real-time EV demand, and storage constraints, highlighting the interdisciplinary nature of hydrogen technology in modern EEE applications.

Electrical and Electronics Engineering (EEE) Perspective

1. Power Conditioning and Control in Electrolyzers

Electrolyzers require stable and precise electrical inputs to operate efficiently and safely. Power conditioning systems—including AC/DC converters, inverters, and voltage regulators—ensure that fluctuating input from renewable sources is converted into a stable, controllable power supply. Advanced control strategies are employed to optimize hydrogen production, minimize energy losses, and prevent damage to electrolyzer components. From an EEE standpoint, real-time monitoring, dynamic load management, and fault detection are crucial for integrating electrolyzers with both the electrical grid and EV charging infrastructure, enabling flexible, demand-responsive hydrogen production.

2. BMS for Hydrogen Storage Systems in EVs

Battery Management Systems (BMS) play a critical role in managing hydrogen storage in fuel cell electric vehicles (FCEVs) and hybrid battery–hydrogen systems. A BMS monitors state-of-charge (SOC), state-of-health (SOH), temperature, and pressure of hydrogen storage tanks to ensure safe operation. It coordinates the flow of energy between batteries and fuel cells, balancing power demands during acceleration, regenerative braking, and long-range cruising. Effective BMS design is essential to protect fuel cells from hydrogen supply fluctuations, maintain optimal performance, and extend system longevity.

3. Integration of Hydrogen Fuel Cells with EV BMS

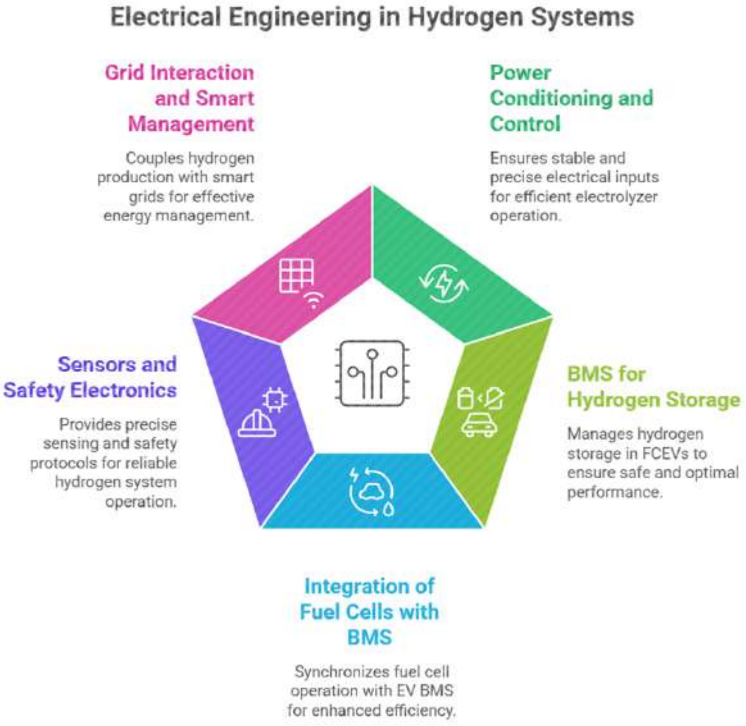
Fuel cell stacks convert hydrogen into electricity, which can be directly fed into the EV powertrain or stored in batteries for peak demand periods. Integration with the EV's BMS ensures synchronized operation, including load sharing between batteries and fuel cells, thermal management, and regenerative energy capture. Advanced control algorithms predict energy needs, optimize hydrogen consumption, and enhance overall vehicle efficiency. This integration represents a critical interface where chemical energy, electrical engineering, and vehicle control converge.

4. Sensors, Monitoring, and Safety Electronics

Hydrogen systems require precise sensing and monitoring for safe and efficient operation. Sensors measure hydrogen pressure, temperature, flow rates, and gas purity, feeding data to control units and BMS algorithms. Safety electronics implement leak detection, automatic shut-off, and emergency venting protocols to mitigate the risks associated with hydrogen's flammability. Integration of such electronics with vehicle and grid control systems enables real-time diagnostics, predictive maintenance, and compliance with safety standards, enhancing reliability in EV and stationary energy applications.

5. Grid Interaction and Smart Energy Management

Hydrogen production and storage can be coupled with smart grids to manage energy supply and demand effectively. Electrolyzers can operate as controllable loads, consuming excess renewable electricity during off-peak periods, while fuel cells can provide power back to the grid during high demand. Advanced energy management systems, combined with BMS and power electronics, enable predictive scheduling, load balancing, and dynamic optimization. This synergy between hydrogen technologies, EV infrastructure, and smart grids illustrates the broader EEE perspective, where electrical engineering solutions maximize the efficiency, safety, and sustainability of hydrogen-based energy systems.



Hydrogen for Electric Vehicles

1. Fuel Cell EVs (FCEVs) vs. Battery EVs (BEVs)

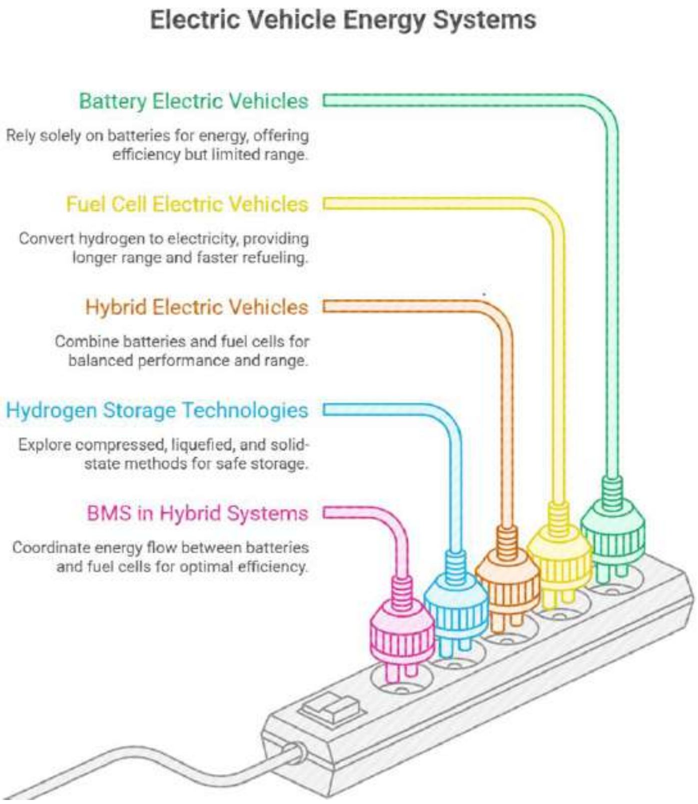
Fuel cell electric vehicles (FCEVs) and battery electric vehicles (BEVs) represent two complementary approaches to electrified transportation. BEVs rely solely on rechargeable batteries to store and deliver energy to the electric drivetrain, offering high energy efficiency and simplicity, but are limited by battery weight, energy density, and charging times. FCEVs, on the other hand, convert hydrogen into electricity using a fuel cell, enabling longer driving ranges and faster refueling. While FCEVs require hydrogen infrastructure and careful energy management, they provide advantages in long-haul transport and scenarios where rapid turnaround is essential. Hybrid approaches combine batteries with fuel cells, leveraging the high-power density of batteries for acceleration and the long-range capability of hydrogen fuel cells.

2. Hydrogen Storage Technologies: Compressed, Liquefied, Solid-State

Safe and efficient hydrogen storage is critical for vehicular applications. Compressed hydrogen is stored at high pressures (350–700 bar) in reinforced tanks, offering compactness and relatively mature technology. Liquefied hydrogen stores hydrogen at cryogenic temperatures (around −253 °C), achieving higher energy density but requiring complex insulation and handling systems. Solid-state storage, using metal hydrides or chemical carriers, enables safer and potentially more compact storage by absorbing hydrogen into a solid matrix, though challenges in kinetics and cost remain. The choice of storage technology directly affects vehicle design, energy management, and integration with BMS and power electronics.

3. Role of BMS in Hybrid Battery–Hydrogen Systems

In hybrid systems combining batteries and fuel cells, the Battery Management System (BMS) plays a central role in coordinating energy flow. It monitors the state-of-charge, temperature, and health of both batteries and hydrogen storage units, dynamically distributing power to optimize efficiency and performance. During peak load events, the BMS ensures batteries provide rapid power, while fuel cells maintain sustained energy supply. It also safeguards against overcharging, deep discharge, and thermal hazards, while enabling predictive control to extend system longevity. Effective BMS integration is essential for achieving the reliability and safety standards required in commercial EV applications.



4. Case Studies of Hydrogen Integration in EVs

Several commercial and pilot projects demonstrate the viability of hydrogen integration in EVs. For example, the Toyota Mirai and Hyundai Nexo employ PEM fuel cells with high-pressure hydrogen tanks, providing ranges comparable to internal combustion vehicles and rapid refueling times. Hybrid approaches, such as fuel cell buses and trucks, integrate onboard batteries with fuel cells to manage power demands efficiently. These case studies highlight how BMS, power electronics, and hydrogen storage technologies converge to deliver safe, high-performance vehicles. They also underscore the potential for hydrogen to complement battery-electric systems, particularly in heavy-duty, long-range, and high-utilization transport applications.

Challenges and Opportunities

1. Cost, Scalability, and Infrastructure Issues

One of the primary challenges in hydrogen adoption is the high cost of production, storage, and distribution compared to conventional fuels and battery-electric systems. Electrolyzers, fuel cells, and high-pressure storage tanks require significant capital investment, and green hydrogen produced from renewable sources remains more expensive than gray or blue hydrogen. Scalability is another concern; building sufficient production capacity and nationwide refueling infrastructure to support widespread fuel cell EV deployment demands coordinated investment and long-term planning. Moreover, hydrogen transport and distribution networks—pipelines, compression stations, and fueling stations—are still underdeveloped, limiting accessibility and efficiency for EV applications.

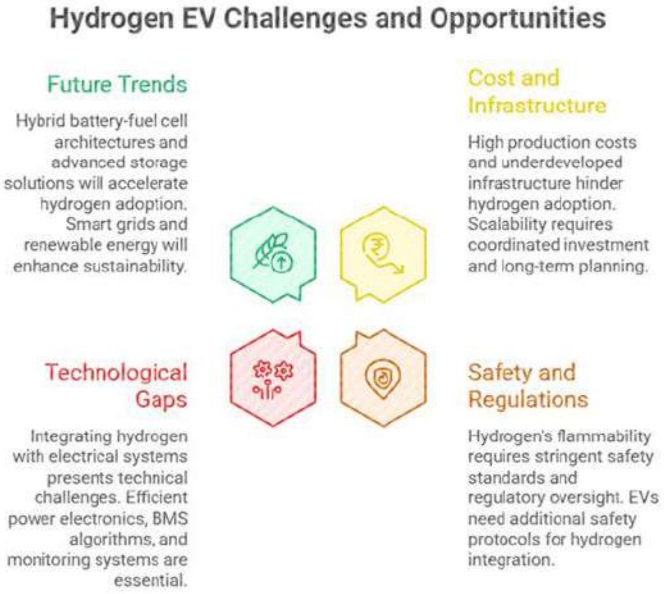
2. Safety and Regulatory Considerations

Hydrogen is highly flammable and has unique handling requirements, making safety a critical concern. Storage tanks, pipelines, and refueling systems must meet stringent regulatory standards to prevent leaks, explosions, and material degradation. For EVs, additional safety protocols are required to integrate hydrogen storage with onboard battery systems, power electronics, and BMS. Governments and standardization bodies are actively developing regulations and certifications to address these risks, ensuring public safety and fostering confidence in hydrogen technologies.

3. Technological Gaps in EEE Integration

Integrating hydrogen production, storage, and fuel cells with electrical and electronic systems presents several technical challenges. Efficient power electronics, advanced BMS algorithms, and real-time monitoring systems are essential to manage energy flows between renewable sources, electrolyzers, batteries, and fuel cells. Current gaps include limitations in dynamic response of electrolyzers to variable renewable input, optimization of hybrid battery–hydrogen systems, and cost-effective sensor networks for safety and performance monitoring. Addressing these gaps is critical for seamless EV operation and maximizing the synergy between chemical and electrical energy systems.

4. Future Trends in EV–Hydrogen Synergy



Future Trends

Hybrid battery-fuel cell architectures and advanced storage solutions will accelerate hydrogen adoption. Smart grids and renewable energy will enhance sustainability.

Cost and Infrastructure

High production costs and underdeveloped infrastructure hinder hydrogen adoption. Scalability requires coordinated investment and long-term planning.

Technological Gaps

Integrating hydrogen with electrical systems presents technical challenges. Efficient power electronics, BMS algorithms, and monitoring systems are essential.

Safety and Regulations

Hydrogen's flammability requires stringent safety standards and regulatory oversight. EVs need additional safety protocols for hydrogen integration.

The convergence of hydrogen and EV technologies is poised to accelerate with advancements in materials, system design, and smart control systems. Emerging trends include hybrid battery–fuel cell architectures, high-efficiency PEM and solid oxide electrolyzers, and solid-state hydrogen storage solutions for compact and safe EV integration. Integration with smart grids and renewable energy sources will further enhance the sustainability and flexibility of hydrogen-powered transport. As BMS and power electronics evolve, predictive energy management and autonomous control will allow real-time optimization of vehicle performance, extending range, reducing costs, and enabling widespread adoption of hydrogen in mobility and energy systems.

Conclusion

1. Summary of Key Technologies

Hydrogen production technologies have evolved from conventional hydrocarbon-based methods, such as steam methane reforming, partial oxidation, and coal gasification, to cleaner and more sustainable approaches like water electrolysis, photocatalytic splitting, and plasma-assisted processes. Electrolytic technologies including alkaline, PEM, and solid oxide electrolyzers offer scalable and low-emission pathways, particularly when integrated with renewable energy sources. Advanced storage methods, such as compressed, liquefied, and solid-state hydrogen, complement these production technologies, enabling practical deployment in fuel cell electric vehicles (FCEVs) and hybrid battery hydrogen systems. Across these technologies, electrical and electronics engineering (EEE) innovations including power conditioning, BMS, sensors, and smart energy management play a pivotal role in ensuring efficiency, safety, and system reliability.

2. Potential of Hydrogen in the EV and EEE Ecosystem

Hydrogen has the potential to transform the EV and broader energy landscape by addressing key limitations of battery-electric vehicles, such as limited driving range and long refueling times. Fuel cells provide high energy density on-demand electricity, while hybrid battery–hydrogen systems enable optimized power delivery, regenerative energy management, and improved system longevity. Integration with EEE solutions allows for intelligent energy control, grid interaction, and safety monitoring, making hydrogen a critical enabler of sustainable mobility and smart energy systems. When coupled with renewable electricity and advanced BMS architectures, hydrogen can significantly contribute to de-carbonization and energy resilience.

3. Research Directions and Outlook

Future research is expected to focus on improving efficiency, durability, and cost-effectiveness of electrolyzers and fuel cells, developing high-density and safe hydrogen storage solutions, and advancing power electronics and BMS integration for hybrid systems. Emerging areas such as photocatalytic water splitting, microbial electrolysis, and solid-state hydrogen storage hold promise for sustainable, decentralized hydrogen production. Furthermore, the convergence of hydrogen technologies with smart grids, EV charging infrastructure, and artificial intelligence-driven energy management will accelerate adoption and optimize system-level performance. Overall, hydrogen represents a transformative pathway in the energy transition, bridging chemical science innovations with electrical engineering and mobility applications to create a cleaner, smarter, and more sustainable future.

References

1. Mohd F. A. Kamaroddin et al., Membrane Based Electrolysis for Hydrogen Production: A Review, Membranes, 11(11):810, 2021. DOI: 10.3390/membranes11110810
2. Ibrahim B. Mansir, A review of hydrogen production and storage technologies for power system integration and applications, Global Energy Interconnection, in press, 2026. DOI: 10.1016/j.gloei.2026.01.001
3. Hydrogen electrolyser technologies and their modelling for sustainable energy production: A comprehensive review and suggestions, International Journal of Hydrogen Energy, 48(72):27841–27871, 2023. DOI: 10.1016/j.ijhydene.2023.04.014
4. Sustainable hydrogen energy fuel cell electric vehicles: A critical review of system components and innovative development recommendations, Renewable and Sustainable Energy Reviews, 215:115601, 2025. DOI: 10.1016/j.rser.2025.115601

Frontiers in Chemical Science

ISBN: 978-93-49938-06-9| Year: 2026 | pp: 70 – 82 |

Carbon Nano Material and Graphene Chemistry

Srimathi. M

S. Dorothy

Department of Chemistry, AMET University, Chennai 603112, Tamil Nadu, India

Email: srimathi2025@ametuniv.ac.in

Article DOI Link: https://zenodo.org/uploads/19637730

DOI: 10.5281/zenodo.19637730

Abstract

The chemistry of carbon nanomaterials and graphene has proven to be one of the most revolutionary in the contemporary materials science due to their outstanding structural, electronic, mechanical, and chemical characteristics. Due to the extensive number of electrochemical properties contains hybridization states SP, SP2, and SP3 the number of nanostructured carbon materials is extensive, including fullerenes, carbon nanotubes (CNTs), graphene, graphene oxide (GO), and reduced graphene oxide (rGO) of these, graphene, the two-dimensional (2D), sp2-hybridized carbon atom in a honeycomb structure, has received more attention than any other material in terms of its extraordinary conductivity to electricity, large surface area, stunning thermal conductivity and mechanical strength. The current developments of graphene chemistry have been on scalable method of synthesizing the materials, surface functionalization heteroatom doping and hybrid nanocomposites to customize the material properties to a desired application. Carbon nanomaterials show a huge promise in various applications in energy storage (supercapacitors, batteries), environmental remediation (adsorption and photocatalysis), biomedical engineering (drug delivery, biosensors), and nano electronics. Moreover, the chemical functionalization of the material based on graphene increases their reactivity, dispersibility and compatibility with polymers and inorganic materials, which increases their applications.

Keywords: Carbon nanomaterials, Graphene-chemistry, Graphene oxide (GO), Reduced graphene oxide (rGO), Carbon nanotubes (CNTs),

Introduction

Carbon nanomaterials are a special category of innovated materials with dimensions of nanoscale and remarkable physicochemical characteristics due to quantum confinement effects and large surface-volume ratios. The research of novel allotropes of carbon, including high tensile strength fullerenes and carbon nanotubes in 1985 and 1991 respectively, and graphene in 2004 have brought because of its atomically thin structure as well as construct of number of other carbon nanostructure characteristics that are attributed to the SP2 carbon networks (Yadav and Awasthi 2022) graphene sheets are wrapped into a cylinder (1-100 nm diameter), and are either metallic or semiconducting, and their chirality (armchair, zigzag, or chiral) determines their behaviour and materials depend on the π-π interactions, edge states and basal plane reactivity with an electron mobility of more than forth a revolution in the nanoscience and nanotechnology (Castro Neto et al. 2009; Zhao et al. 2021). Of them, the most important graphene is a building block of other carbon nanostructures, are graphite (layered sheets of graphene), CNTs (rolled sheets of graphene), and fullerenes (closed graphene cages). Arrangement of graphene is a single sheet of carbon atoms are closely stacked two-dimensional structure (2-D) of honey comb hexagonal lattices with outstanding characteristics of high electron mobility outstanding mechanical strength, and exceptional thermal conductivity (Kasálková et al. 2021). These characteristics render graphene an excellent choice of the next generation electronic devices, flexible materials and high-performance composites because of high carrier mobility, large surface area, thermal conductivity which make it a platform of high versatility in terms of advanced applications. Nevertheless, pure graphene is chemically inactive and has no bandgap that restricts its immediate use in some electronic and catalytic applications. To address these shortcomings, graphene has received a lot of research on its chemical modification and functionalization (Sastry, Panjikar, and Raman 2021). The changes allow the graphene-based materials to react with the pollutants, biomolecules, and electroactive species. Recent studies have involved the development of the hybrid nanocomposites involving graphene with metal oxides, polymers and other nanomaterials to address the inherent drawbacks like aggregation and few active sites (Potbhare et al. 2024). These composites are more superior in terms of performance in catalysis, sensing as well as in energy applications because of the synergistic effects (Ayanda et al. 2024). Meanwhile, graphene is a perfect two-dimensional(2-D) support of metal oxides, polymers and enzyme dispersion avoiding aggregation and increasing interfacial charge transfer. CNTs, rolled sheets of graphene, in parallel have much in common with graphene except that they have a higher anisotropy, chirality dependent electronic properties, and higher aspect ratios (Yang et al. 2020). CNTs and graphene when combined into hybrid structures (e.g. graphene CNT aerogels, bucky papers, and 3-D scaffolds) have resulted in materials with synergistic mechanical, electrical and transport properties as electrodes, structural composite and membrane (Yang et al. 2020). It is over this context that the current work will attempt to give a unified discussion on the chemistry of the carbon nanomaterial, and graphene with special attention to the interaction between the structure of the atoms, the synthetic pathway, chemical modification, and macroscopic functional performance (Sheoran et al. 2022). Simultaneously, CNTs and fullerenes are the other carbon nanomaterials, which also play an important role in the development of nanotechnology. In recent times, the topic of sustainable and scalable synthesis schemes of carbon nanomaterials has gained more and more attention, and such schemes are chemical vapor deposition (CVD), electrochemical exfoliation, and green synthesis. Moreover, application is graphene-related materials in the real-life systems, especially water purification, pollutant degradation, biosensing and energy devices have proved their usefulness to the real world (Saleh and Hassan 2023). Although these have been greatly improved, a number of challenges still exist as large scale production, cost effectiveness, structural defect and environmental concern. The solutions to these problems are critical in commercialising and popularisation of carbon nanomaterials. Generally, carbon nanomaterials and graphene chemistry remain on the tip of the scientific innovation and promise enormous opportunities in the next few decades in terms of interdisciplinary research and technological progress (Zhan et al. 2025).

This chapter provides a critical view of the way to fabricated graphene chemistry to address the need of the upcoming technologies by incorporating the recent advances of the 2020-2026.

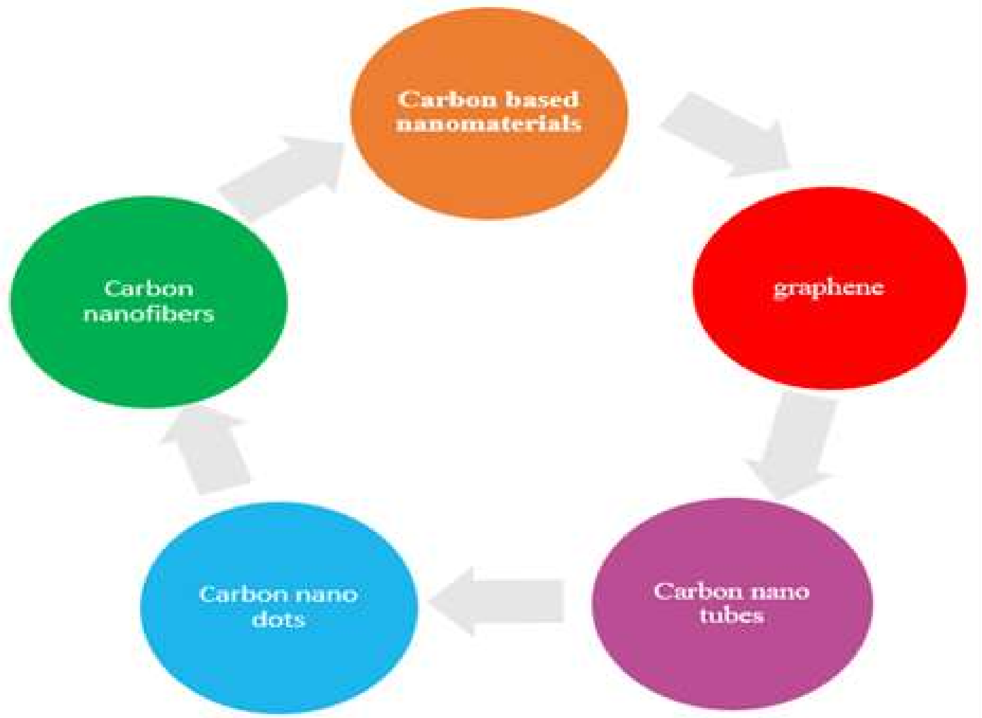


Fig 1 represents the classification of carbon-based nanomaterials

Objectives

- The overall goal of this chapter is to give a systematic and chemistry-based discourse of the carbon nanomaterials, and specifically the graphene and its derivatives. The particular objectives are formulated in the manner below.
- To develop the bonding and design of carbon nanomaterials in constituents of the sp2 carbon framework presently occurring in graphene, CNTs and other different nanocarbon structures, and to acquire insight into how extent and superb govern the significant physical properties (Burkholder et al. 2022).
- To the major synthesis routes to graphene and CNTs, including mechanical exfoliation, chemical oxidation reduction, chemical vapor deposition (CVD), epitaxial growth on silicon carbide (SiC) and electrochemical methods and comment on the impact of each of the method on defect density, oblique dimension and chemical functionalization (Hutapea et al. 2025).
- To inspect of finding of graphene chemistry to property engineering, such as covalent and non-covalent nature, defect-site engineering to avoid these issues, doping with heteroatom, design of surface functional groups and to develop the overall structure, property, and functional performance relationship (Narayan and Bezborah 2024).
- To assess the performance of the graphene based nanocomposites in realistic areas of application, e.g. energy storage (batteries and supercapacitors), electrocatalysis (oxygen reduction, CO2 reduction), photocatalysis, and polymer reinforced nanocomposites, by observing experimental result and structure performance determine the existing barriers and future drift, such as scalability, reproducibility, environmental problems, and poison damage, and appeal of machine learning supported design to graphene chemistry, and with the belief of notify rational plan of material development. The realization of such goals will provide the reader with an insight to how chemical design at the nanoscale, and not simply taking the form of graphene as a magic filler, can be exploited to realize customized, high-performance carbon nanomaterials the advanced technological platform. The key goals of the research in the area of carbon nanomaterial and graphene chemistry are complicated, this is why the simple knowledge is combined with the technological application.

Data and Methodology

There are numerous methods to synthesize graphene via top down and bottom-up methods and the methods have different implications depending on their size, defect density, and chemical functionality (Narayan and Bezborah 2024). The rGO was obtained through chemical oxidation of graphite (e.g., Hummers modified method) and followed by sonication to produce graphene oxide (GO) dispersions and followed by thermal or chemical reduction. Methane or acetylene was used as a source of carbon and deposited onto copper or nickel foils through chemical vapor deposition (CVD) and then shifted to target substrates with the help of polymer10.5772/intechopen.106058. Synthesis of carbon nanotubes is done through: Arc discharge or laser ablation of graphite targets of high quality single walled CNTs (Yogesh et al. 2021). Large quality, few layer graphene flakes with minimal defects and carrier mobility on SiO2 substrates are obtained with mechanical exfoliation (e.g. Scotch tape method) but with low yield, low scalability, and the flakes have different sizes. Conversely, chemical exfoliation of graphene oxide (GO) through Hummers-type oxidation of graphite and subsequent sonication and reduction offers a solution processable, large area graphene like sheets, at higher defect density and oxygen groups, but makes use of a more scalable process (Bastos et al. 2025)through thermal, chemical, or electrochemical processes, the restoration of some SP2 conjugation by removing GO (rGO) cannot be made complete, sacrificing functional groups, and results in the trade of between processability and electrical performance. Most generally used of the bottom-up methods to date is the CVD of graphene films (on transition metal substrates, most commonly Cu and Ni) in large area, continuous films. High temperature thermal deposition of silicon carbide (SiC). Epitaxial growth on silicon carbide (SiC) High quality, wafer scale graphene with low density of defects and good electrical characteristics is obtained by high temperature thermal decay of silicon carbide (SiC) to leave a graphene overlayer. SiC substrates are however very expensive and require high temperature processing making its use difficult to implement more widely. In more recent times, electrochemical exfoliation, laser induced graphitization, as well as, plasma assisted synthesis have been examined to produce high yield and large area graphene with defect densities and edge chemistries, which can be tuned. The chemical reactivity of the graphene is due to the abundant reactivity of its sp2 carbon lattice and edges, which can be altered using covalent, non-covalent and heteroatom doping. The bases planes or edges are usually reacted to covalent functionalization by oxidation, radical addition, or cycloaddition. As an illustration, the use of powerful oxidants e.g. HNO3 /H2SO4 on graphene results in the addition of epoxide, hydroxyl and carboxyl groups to produce graphene oxide (GO) with increased hydrophilicity and solubility (Khine et al. 2022). Further reduction will produce functional groups that remain so that they can act as anchoring sites to metal nanoparticles, polymers, or biomolecules. In a similar fashion, the aromatic molecules e.g. pyrene derivatives may be attached to the graphene, using the π -π interactions, as linkers to further fix the catalysts or biomolecules. Add n type character to improve the catalytic activity of oxygen reduction reactions (ORR) and metal free electrocatalysis. P-type graphene with enhanced mobility of holes due to boron doping, and band bending and interfacial charge transfer can be further controlled by co doping with a variety of hetero-atom. These are the chemical modifications that are of profound implications to both the electronic performance and the catalytic performance. Indicatively GO based materials, on the contrary, are excellent supports of photocatalytic TiO2 nanoparticles, even though they have a greater density of defects that enable the oxygen containing groups to form strong interfacial bonds and charge separation efficiency.

Result and Discussion

Structural framework of carbon nanomaterials and graphene issp2bonded carbon structure, where every carbon atom is trigonally bonded, and provides one electron to a large 3D. This connectivity in graphene gives a 2-D honeycomb sheet with bond length of about 1.42 A and bond angle of about 120 and, therefore, having strong in plane covalent bonding and weak interlayer van der Waals between adjacent layers. Carbon nanotubes may be considered to be cylindrically-shaped rolled sheets of graphene, with the chirality determined by the rolling vector nm. The CNTs are normally single walled (SWCNTs) and those with a diameter of ~0.72-2 nm and length up to several micrometers, and multi walled CNTs (MWCNTs) that are concentric cylinders composed of graphene with much larger diameters. Similar to graphene, CNTs are of high tensile strength, highly electrically conductive and of large surface area although their one-dimensional nature brings significant anisotropy and end effect dependent chemical reactivity. and heteroatom substitution, have a great impact on the electronic structure, mechanical strength, and surface reactivity. As it is stressed in this section, the chemistry of graphene is not just a frivolous overlay, but it is fundamentally related to its topology at the atomic scale and bonding environment (Kim and Kuljanishvili 2023).

1. Common Applications-Based Graphene

This section covers overall applications highlights the different roles of carbon nanomaterials and graphene chemistry across many fields. Their erractic properties and chemistry available transformative impacts on energy, environment, healthcare, and industry, positioning them as cornerstone materials for future technological advancements.

2. Electronics and Flexible Devices

The electrical attribute of graphene such as ultra-large mobility of carriers and ballistic transport of electrons are the basis of future electronics. The field-effect transistors (FETs) using graphene can be used to work at terahertz frequencies and are faster and more efficient than silicon-based devices (Auton et al. 2017). Its 2-D format allows it to come up with ultra-thin, flexible, and transparent touchscreen, display and wearable electronics conductors. Graphene electrodes are better in terms of flexibility and durability than the brittle indium tin oxide (ITO), and are suitable to the future display and flexible sensors (Wang et al. 2021). Graphene Hybrid structures with carbon nanotubes (CNTs) are even better at improving the performance of the device. Graphene-CNTs are high-conductivity interconnects and flexible wiring, which can be used to produce strong, lightweight circuits in portable electronics and aerospace. Radio-frequency identification (RFID), flexible antennas, and other materials based on these materials are also used in the development of the new scope of wireless communication technologies (Zhou et al. 2024).

3. Energy Storage and Conversion

Carbon nanomaterials are also essential in further development of the energy storage technology especially in supercapacitors and lithium-ion batteries. Graphene electrodes in supercapacitors realize particular capacitance of 300-500 F/g which is 2-3 times higher than the traditional activated carbon electrode (Elsehsah, Noorden, and Saman 2024). Graphene aerogels and composites have superior surface area, electrical conductivity and mechanical strength properties and hence allow quick charge-discharge time and stability. Graphene anodes have been shown to have high capacities of up to 800 mAh/g and high retention following thousands of cycles in lithium-ion batteries, which meets the need of a high-energy-density storage. Graphene chemistry is also effective in catalytic processes of energy conversion. The Graphene-bound metal nanoparticles can effectively react to hydrogen evolution and oxygen reduction reaction, which are essential to fuel cells and electrolyzers. Practical Graphene-TiO2 hybrids can reduce CO2 to methane which is five times greater than the pure TiO2, leading to the possibility of using hybrids in the sustainable energy system (Patel et al. 2026).

4. Sensing and Biomedical

Graphene chemistry will provide new opportunities in the field of biomedicine, specifically in the field of drug delivery, biosensing, and imaging. GO and rGO are biocompatible and functionalizable surfaces, which may be used to deliver anticancer drugs and biomolecules to a specific location. Graphene biosensors respond to biomarkers at extremely low concentrations and it enables early diagnosis of diseases and personalized medicine. Based on the non-invasive glucose monitoring of flexible graphene sensors, the wearable technologies of healthcare technologies are developed. Graphene also improves the imaging and diagnostic. The graphene contrast agents enhance the magnetic resonance imaging (MRI) resolutions whereas the graphene quantum dots allow the imaging of fluorescence with high sensitivities. All these applications highlight the fact that graphene could make a revolution in the field of healthcare and diagnostics (Kumar et al. 2023)

5. Photonics and Optoelectronics

Graphene has the advantage of having special optical characteristics that allow it to be used in photonics and optoelectronics. The photodetectors based on graphene are sensitive to a wide range of light including the ultraviolet and the terahertz spectrum, which can be used to create high-rate imaging and communication networks. Graphene plasmonics are useful in the design of miniaturized optical components in integrated circuits, and it outperforms other material. Hybrid graphene-semiconductor systems are also used to improve the light-emitting diodes (LEDs) and solar cells, which increase their efficiency and use less energy. These developments indicate the use of graphene in sustainable energy technologies and

- **Dye Adsorption Mechanisms**

Graphene and its derivatives are characterised by great adsorption properties by π -interaction, electrostatic force and hydrogen bonding. Graphene oxide has an increase in affinity towards dye molecules by the existence of oxygen containing functionality groups in it and minimizes electron -hole recombination in semiconductor photocatalysts. In the recent literature, it is emphasized that, rGO has better adsorption properties because of high porosity, plentiful active sites, tunable surface chemistry. Graphene-CNT composites and graphene-metal oxide nanostructures are some of the examples of hybrid materials that exhibit high adsorption capacity because they have more surface area and synergies composites of graphene and metal oxide like TiO2/GO and ZnO/GO have shown a better photocatalytic activity than the pure semiconductors (Busarello et al. 2023). They cause the formation of reactive oxygen species (ROS) in the form of hydroxyl radicals and superoxide ions which are effective in degrading the dye molecules to harmless products. Doped graphitic carbon nitride (g-C3N4) with almost 100 per cent pollutant degradation in visible light graphene-based heterostructures with orders of magnitude enhancement in catalytic activity and adsorption at the same time CNT/GO composites with simultaneous improvement in catalytic activity and adsorption (Khan et al. 2025).

- **Sensor Applications**

Sensors based on graphene have attracted immense interest as it is very sensitive, selective, and has a quick response. The conductivity and surface area are high allowing detection of gases, biomolecules and pollutants. Recent developments include such as graphene electrochemical sensors, heavy metal sensors and Graphene flexible wearable sensor. biomedical sensors and graphene Optical sensors, graphene quantum dots. The transduction of the graphene functionalized version increases the selectivity and signal transduction and this makes it useful in real time monitoring.

- **Supercapacitors**

Supercapacitors are widely applied using graphene because it has a dominant surface area and conductivity. It allows fast charge-discharge cycles, as well as power density. The latest developments are graphene-based hybrid electrodes consisting of metal oxides and conducting polymers, 3-D graphene architectures with better ion transport flexible and wearable supercapacitors. These systems are characterized by high capacitance, long cycle life and better energy density thus can be used in the next-generation energy storage devices (Ran et al. 2024).

- **Conversion and Storage of Energy**

Graphene is important in energy transformation technology which includes solar cells, fuel cell, hydrogen generation. Innovations: Graphene-based photocatalysts to enhance hydrogen evolution Graphene-based electrode in lithium-ion and sodium-ion batteries enhanced charge transport in solar cells. Graphene composites have an immeasurable effect on efficiency and stability in such systems because of efficiency of movement of electrons and recombination losses are minimized.

- **Antibacterial Activity**

The materials made of graphene have high antibacterial properties because of Physical damage of bacterial cells through disruption of cell membranes Oxidative stress caused by ROS Electron transfer reactions. GO and rGO are especially efficient in terms of Gram-positive and Gram-negative bacteria, which is why they will be applicable in the bio-medical and environmental context (Sandhu et al. 2025)

- **Heavy Metal Adsorption**

The materials made of graphene are effective in elimination of heavy metals including Pb2+, Cd2 +and Cr6+ present in wastewater. These are surface complexation, ion exchange electrostatic interactions. Graphene has a functionalized form, which is more selective and has a higher adsorption capacity therefore, it can be used in the purification of water.

- **Fuel Cell and Batteries**

Graphene finds large application in the fuel cells and batteries because of its good conductivity and stability. Applications Is catalyst support in fuel cell Catalyst support in fuel cells, Electrodes in lithium-ion batteries. Graphene-based solid-state batteries. Recent development is on enhancing the energy density, life cycle and safety by using graphene-based nanocomposites (Shankar et al. 2023).

Conclusion

In this chapter, carbon nanomaterial and graphene chemistry provide conclusion in the form of elloborate paragraph. Carbon nanomaterials and graphene chemistry have become pillars of transformational materials science today, with unparalleled opportunities in the environmental, energy and biomedical fields. The unusual physico-chemical characteristics of graphene and with carbon nanostructures, also high surface area, electrical conductivity, mechanical strength, and adjustable surface properties, have made them greatly applicable in large-technology areas. These materials are very useful in photocatalytic degradation of dyes that lead to high charge separation efficiency and light absorption, which are useful in increasing degradation rates of organic pollutants. Correspondingly, their exceptional adsorption capacity, and surface reactivity render them very useful in eliminating dye and sequestration of heavy metal ions to solve serious environmental cleanup issues. Graphene-based nanomaterials have been shown to be extremely sensitive, selective, and fast responding in sensing with a high rate of electron mobility and active surface area, which makes them suitable to detect gases, biomolecules, and toxic substances. Moreover, their incorporation into energy storage and conversion systems including supercapacitors, lithium-ion batteries, and fuel cells has contributed to higher energy density, charge-discharge rates and extensive cycling durability. These innovations play an important role in the creation of efficient and sustainable energy technologies. Also, the characteristics of the antibacterial effect of graphene derivatives due to the membrane disruption effect and the oxidative stress effect have provided new opportunities in the field of biomedical and healthcare use. Along with these encouraging developments, there are a number of issues such as scale synthesis, cost-efficiency, stability of the material, and possible environmental and health outcomes. The solution to these problems has to do with further interdisciplinary studies that are aimed at green synthesis strategy, functionalization of nanoparticles, and lifecycle evaluation. Generally, carbon nanomaterials and graphene chemistry is a very dynamic and highly influential field of study, and it has the potential to transform various sectors and play a significant role in global sustainability and technological advancement.

References

1. Auton, Gregory, Dmytro B. But, Jiawei Zhang, Ernie Hill, Dominique Coquillat, Christophe Consejo, Philippe Nouvel, Wojciech Knap, Luca Varani, Frederic Teppe, Jeremie Torres, and Aimin Song. 2017. “Terahertz Detection and Imaging Using Graphene Ballistic Rectifiers.” Nano Letters 17(11):7015–20. doi: 10.1021/ACS.NANOLETT.7B03625.
2. Ayanda, Olushola Sunday, Augusta Oluchi Mmuoegbulam, Onyemaechi Okezie, Naseer Inuwa Durumin Iya, Sa’adatu Eri Mohammed, Philip Hegarty James, Abba Bashir Muhammad, Augustine Agorye Unimke, Sabur Ajibola Alim, Sharhabil Musa Yahaya, Ayomipo Ojo, Toyin Olanike Adaramoye, Stella Kemilola Ekundayo, Aminu Abdullahi, and Hamza Badamasi. 2024. “Recent Progress in Carbon-Based Nanomaterials: Critical Review.” Journal of Nanoparticle Research 26(5). doi: 10.1007/S11051-024-06006-2.
3. Bastos, Tarso Leandro, Camila Cristina da Silva, Daniela Nunes, Elvira Fortunato, Rodrigo Martins, Devadharshini Kathan, William Earl Mustain, Rogério Valentim Gelamo, and Flavio Colmati. 2025. “Metal-Free Multilayer Graphene Electrodes Activated by PECVD for Electrochemical Oxidation

Enhancement." ACS Applied Nano Materials 8(47):22586–604. doi: 10.1021/ACSANM.5C03602.

4. Burkholder, Michael B., Fahim Bin Abdur Rahman, Edward H. Chandler, J. R. Regalbuto, B. F. Gupton, and J. Meynard M. Tengco. 2022. "Metal Supported Graphene Catalysis: A Review on the Benefits of Nanoparticular Supported Specialty Sp2 Carbon Catalysts on Enhancing the Activities of Multiple Chemical Transformations." Carbon Trends 9. doi: 10.1016/J.CARTRE.2022.100196.
5. Busarello, Pamela, Samara de Quadros, Lizandra M. Zimmermann, and Eduardo G. C. Neiva. 2023. "Graphene Oxide/ZnO Nanocomposites Applied in Photocatalysis of Dyes: Tailoring Aqueous Stability of Quantum Dots." Colloids and Surfaces A: Physicochemical and Engineering Aspects 675:132026. doi: 10.1016/J.COLSURFA.2023.132026.
6. Castro Neto, A. H., F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim. 2009. "The Electronic Properties of Graphene." Reviews of Modern Physics 81(1):109. doi: 10.1103/RevModPhys.81.109.
7. Elsehsah, Khaled Abdou Ahmed Abdou, Zulkarnain Ahmad Noorden, and Norhafezaidi Mat Saman. 2024. "Graphene Aerogel Electrodes: A Review of Synthesis Methods for High-Performance Supercapacitors." Journal of Energy Storage 97. doi: 10.1016/J.EST.2024.112788.
8. Hutapea, Joys Alisa Angelina, Yosia Gopas Oetama Manik, Sun Theo Constan Lotebulo Ndruru, Jingfeng Huang, Ronn Goei, Alfred Iing Yoong Tok, and Rikson Siburian. 2025. "Comprehensive Review of Graphene Synthesis Techniques: Advancements, Challenges, and Future Directions." Micro 2025, Vol. 5, Page 40 5(3):40. doi: 10.3390/MICRO5030040.
9. Kasálková, Nikola Slepičková, Petr Slepička, Václav Švorčík, Inmaculada Rodríguez-Ramos, and Marwan Al-Haik. 2021. "Carbon Nanostructures, Nanolayers, and Their Composites." Nanomaterials 2021, Vol. 11, Page 2368 11(9):2368. doi: 10.3390/NANO11092368.
10. Khan, Muhammad Asim, Sadaf Mutahir, Imrana Shaheen, Yuan Qunhui, Mohamed Bououdina, and Muhammad Humayun. 2025. "Recent Advances over the Doped G-C3N4 in Photocatalysis: A Review." Coordination Chemistry Reviews 522:216227. doi: 10.1016/J.CCR.2024.216227.
11. Khine, Yee Yee, Xinyue Wen, Xiaoheng Jin, Tobias Foller, and Rakesh Joshi. 2022. "Functional Groups in Graphene Oxide." Physical Chemistry Chemical Physics 24(43):26337–55. doi: 10.1039/D2CP04082D.
12. Kim, Yoosuk, and Irma Kuljanishvili. 2023. "Recent Advances in Carbon Nanotube Patterning Technologies for Device Applications." Frontiers in Carbon 2:1288912. doi: 10.3389/FRCRB.2023.1288912.
13. Kumar, Rajesh, Dinesh Pratap Singh, Romina Muñoz, Mongi Amami, Rajesh Kumar Singh, Shipra Singh, and Vinod Kumar. 2023. "Graphene-Based

Materials for Biotechnological and Biomedical Applications: Drug Delivery, Bioimaging and Biosensing.” Materials Today Chemistry 33:101750. doi: 10.1016/J.MTCHEM.2023.101750.

14. Narayan, Jyoti, and Kangkana Bezborah. 2024. “Recent Advances in the Functionalization, Substitutional Doping and Applications of Graphene/Graphene Composite Nanomaterials.” RSC Advances 14(19):13413–44. doi: 10.1039/D3RA07072G.
15. Patel, Abhishek R., Anas D. Fazal, Trupti D. Solanky, Subhendu Dhibar, Sumit Kumar, and Sumit Kumar Panja. 2026. “Recent Advances and Challenges in Graphene-Based Nanomaterials for Photocatalytic CO2 Reduction.” Materials Advances 7(1):109–43. doi: 10.1039/D5MA00750J.
16. Potbhare, Ajay K., S. K. Tari. Aziz, Mohd Monis Ayyub, Aniket Kahate, Rohit Madankar, Sneha Wankar, Arnab Dutta, Ahmed Abdala, Sami H. Mohmood, Rameshwar Adhikari, and Ratiram G. Chaudhary. 2024. “Bioinspired Graphene-Based Metal Oxide Nanocomposites for Photocatalytic and Electrochemical Performances: An Updated Review.” Nanoscale Advances 6(10):2539–68. doi: 10.1039/D3NA01071F.
17. Ran, Jing, Yafei Liu, Huixia Feng, Haixiong Shi, and Qing Ma. 2024. “A Review on Graphene-Based Electrode Materials for Supercapacitor.” Journal of Industrial and Engineering Chemistry 137:106–21. doi: 10.1016/J.JIEC.2024.03.043.
18. Saleh, Hosam M., and Amal I. Hassan. 2023. “Synthesis and Characterization of Nanomaterials for Application in Cost-Effective Electrochemical Devices.” Sustainability 2023, Vol. 15, Page 10891 15(14):10891. doi: 10.3390/SU151410891.
19. Sandhu, Zeshan Ali, Muhammad Asam Raza, Kainat, Farhana Aman, Muhammad Sami Arshid, Syeda Dure Kashf Jaffary, Sehar Arshad, Mustafa Raza, Abdullah G. Al-Sehemi, and Necmi DEGE. 2025. “Graphene-Metal Oxide Nanocomposites: Empowering Next-Generation Energy Storage Devices.” Materials Science and Engineering: B 313:117947. doi: 10.1016/J.MSEB.2024.117947.
20. Sastry, Shiva Shahriari Murali, Santosh Panjikar, and RK Singh Raman. 2021. “Graphene and Graphene Oxide as a Support for Biomolecules in the Development of Biosensors.” Nanotechnology, Science and Applications 14:197–220. doi: 10.2147/NSA.S334487.
21. Shankar, Krishna, Satakshi Agarwal, Subham Mishra, Pranshul Bhatnagar, Sufiyan Siddiqui, and Iyman Abrar. 2023. “A Review on Antimicrobial Mechanism and Applications of Graphene-Based Materials.” Biomaterials Advances 150:213440. doi: 10.1016/J.BIOADV.2023.213440.
22. Sheoran, Karamveer, Harjot Kaur, Samarjeet Singh Siwal, Adesh Kumar Saini, Dai Viet N. Vo, and Vijay Kumar Thakur. 2022. “Recent Advances of Carbon-

Based Nanomaterials (CBNMs) for Wastewater Treatment: Synthesis and Application." Chemosphere 299:134364. doi: 10.1016/J.CHEMOSPHERE.2022.134364.

23. Wang, Tingting, Kuankuan Lu, Zhuohui Xu, Zimian Lin, Honglong Ning, Tian Qiu, Zhao Yang, Hua Zheng, Rihui Yao, and Junbiao Peng. 2021. "Recent Developments in Flexible Transparent Electrode." Crystals 2021, Vol. 11, Page 511 11(5):511. doi: 10.3390/CRYST11050511.
24. Yadav, Thakur Prasad, and Kalpana Awasthi. 2022. "Carbon Nanomaterials: Fullerene to Graphene." Transactions of the Indian National Academy of Engineering 7(3):715–37. doi: 10.1007/s41403-022-00348-w.
25. Yang, Feng, Meng Wang, Daqi Zhang, Juan Yang, Ming Zheng, and Yan Li. 2020. "Chirality Pure Carbon Nanotubes: Growth, Sorting, and Characterization." Chemical Reviews 120(5):2693–2758. doi: 10.1021/ACS.CHEMREV.9B00835.
26. Yogesh, Gaurav Kumar, Shivam Shukla, D. Sastikumar, and Pankaj Koinkar. 2021. "Progress in Pulsed Laser Ablation in Liquid (PLAL) Technique for the Synthesis of Carbon Nanomaterials: A Review." Applied Physics A 2021 127:11 127(11):810-. doi: 10.1007/S00339-021-04951-6.
27. Zhan, Meiqiu, Minjie Xu, Weijun Lin, Haijie He, and Chuang He. 2025. "Graphene Oxide Research: Current Developments and Future Directions." Nanomaterials 2025, Vol. 15, Page 507 15(7):507. doi: 10.3390/NANO15070507.
28. Zhao, Biao, Shenghua Yang, Jianping Deng, and Kai Pan. 2021. "Chiral Graphene Hybrid Materials: Structures, Properties, and Chiral Applications." Advanced Science 8(7):2003681. doi: 10.1002/ADVS.202003681; PAGEGROUP: STRING: PUBLICATION.
29. Zhou, Xinyao, Ting Leng, Kewen Pan, Yang Liu, Zirui Zhang, Jiashen Li, Kostya S. Novoselov, and Zhirun Hu. 2024. "A Sustainable Approach towards Printed Graphene Ink for Wireless RFID Sensing Applications." Carbon 218:118693. doi: 10.1016/J.CARBON.2023.118693.

Frontiers in Chemical Science

ISBN: 978-93-49938-06-9| Year: 2026 | pp: 83 – 91 |

Carbon Nanomaterials and Graphene Chemistry

Next-generation Graphene Derivatives for Detoxification of Heavy Metals from Wastewater

[1]Ms. Jeevitha R

[2]Dr. Dorothy S

[1]Research Scholar, Department of Chemistry, AMET University, Chennai, India

[2]Assistant Professor, Department of Chemistry, AMET University, Chennai, India

Email: jeevitharajkumar10924@ametuniv.ac.in

Article DOI Link: https://zenodo.org/uploads/19637854

DOI: 10.5281/zenodo.19637854

Abstract

In recent years several carbon materials are emerging, among them graphene and their derivatives are attracted, due to their high surface area, chemical stability, and thermal conductivity. Graphene derivatives, Graphene oxide (GO), reduced graphene oxide (rGO) are obtained from graphite by Hummers method. Graphite powder is allowed to combine with KMnO4, NaNO3, and con.H2SO4 to synthesis GO sheets. The formed GO are addition to reducing agents produces rGO. This is a rapid synthesis, higher yield method and got good quality of GO, rGO nanosheets. These nanoshests (GO, rGO) act as adsorbents in waste water, comes out from industries contains toxic heavy metals such as Cu2+, Pb2+, Zn2+, U2+, etc., are removed. The present chapter, especially discusses, synthesis method, adsorption of heavy metals, mechanisms, future outlook of graphene derivatives, and the detoxification of water containing toxic heavy metals.

Keywords: waste water treatment, detoxification, graphene oxide (GO), reduced graphene oxide (rGO).

Introduction

Water is the universal solvent used in industries such as pharmaceuticals, mining, textiles, leather, food, etc., often containing dyes, pesticides, heavy metals (Cu2+, Pb2+, Zn2+, Cd2+, Hg2+, As3+, As5+, and Cr6+), which are extremely toxic to the ecological systems and human health, due to these factors industries requires detoxification of heavy metals from the water bodies. Numerous technologies are deployed including ion exchange, membrane-based filtration, electrolysis, adsorption, flocculation, precipitation, and osmosis are usually characterized by shortcomings that include failure to eliminate all the contaminants, high costs of operation, sludge production, and secondary pollution. Therefore, there is an urgent necessity of the development of high-tech, sustainable and highly efficient materials with selective and fast heavy metal removal. Among them adsorption is a feasible, low-cost method because of the physiochemical characteristics to separate the toxic metals. In this process various adsorbents have been investigated for the detoxification of toxic metals, such as layered double hydroxide (LDH), activated carbon, chalcogenides, polymeric materials, clays, zeolites, magnetic materials and allotropic forms of carbon materials (carbon nanotubes [CNT's], carbon nano-spheres, activated carbon, graphene, GO, rGO)(Ain, Farooq, & Jalees, 2020; Sadeghi, Tofighy, & Mohammadi, 2020).

In this regard, graphene and its future generation forms have become potential solutions in the use of graphene in environmental remediation. Graphene is a two-dimensional (2D) film of sp2 hybridized carbon atoms in the form of a hexagonal lattice with outstanding physicochemical characteristics such as a high specific surface area (~2630 m2/g), very high electrical conductivity, mechanical strength and surface chemistry which can be tuned (Viprya, Kumar, & Kowshik, 2023). Nonetheless, pure graphene is quite inert and it has no functional groups to interact with the heavy metal ions. To eliminate these shortcomings, different forms of graphene including graphene oxide (GO), reduced graphene oxide (rGO), functionalized graphene, heteroatom-doped graphene and graphene-based hybrid nanocomposites have been produced.

In the case of Graphene oxide, the oxide has numerous oxygenated functional groups (hydroxyl, epoxy and carboxyl) and they are used as active sites in the adsorption of metal ions via electrostatic interactions, complexation and ion exchange mechanisms. Reduced graphene oxide although has fewer oxygen groups is the one that has better conductivity and structural stability and can be used in composites with metal oxides, polymers as well as layered double hydroxides (LDHs). The current developments have been centered on the next-generation derivatives of graphene, such as nitrogen-doped graphene, sulfur-functionalized graphene, magnetic graphene composite, and bio-inspired graphene hybrids, which are better adsorbents with high selectivity and recyclability.

In this chapter the high-tech materials allow the following processes used to remove heavy metals, including surface adsorption, redox reactions, photocatalytic reduction, and hybrid system interactions. They can be used to remove select contaminants with their tunable physicochemical properties in different conditions within the environment. Consequently, the use of graphene-based materials is becoming a promising effective material, economically viable, and non-polluting ways of treating wastewater.

Objectives

The preliminary objective of this chapter are

- To explain the synthesis of graphene and their derivatives
- To illustrate the adsorption of heavy metals and mechanisms
- To analyze the efficiency of the adsorbents
- To highlight the challenges and future perspective

Methodology

1. Graphene Derivatives Synthesis

The introduction of graphene sheets in 2004 by Geim and Novoselov, graphene, composed of conjugated sp2 carbon atoms, for the next generation material for many applications, such as energy storage, sensors, adsorption, electrochemical and nano-electronic applications. Fabricated of graphene oxide by Brodie method (HNO_3 oxidation), Staudenmaier method and Hummers method. (Mohammed et al., 2024) studied that most frequently used methods are hummers method and altered hummers methods Here, a graphite powder undergoes oxidation by the use of effective oxidizing agents like potassium permanganate ($KMnO_4$) in concentrated sulfuric acid (H_2SO_4) in the presence of sodium nitrate ($NaNO_3$). The oxidation reaction makes the layer of graphite to contain oxygen-based functional groups (carboxyl, hydroxyl, carbonyl and alkoxyl), which results in the development of graphene oxide sheets. The resulting GO is subsequently exfoliated by way of ultra-sonication to get single or few layer nanosheets. While GO undergoes reduction either by thermal, chemical or electrochemical to form reduced graphene oxide. The reducing agents used in chemical reduction include hydrazine hydrate, sodium borohydride ($NaBH_4$), or ascorbic acid but thermal reduction is realized by heating GO in an inert atmosphere. Plant extracts or biomolecules have also been considered as a source of green reduction method as they are environmentally friendly.

2. Hybrid Nanocomposite Synthesis

Graphene derivatives are frequently functionalized or embedded in hybrid nanocomposites in order to improve the adsorption processes. The covalent or non-covalent modifications can be done to achieve functionalization. Covalent functionalization entails functional grouping of $-NH_2$, -SH or polymers on the graphene surface, and hence an increment in the number of active binding sites by the covalent functionalization of the heavy metal ions. Non covalent mechanisms are π- π interactions, hydrogen bonding forces and van der Waals forces.

Graphene derivatives are used to form hybrid composites with other substances, which include metal oxides (Fe_3O_4, TiO_2, ZnO)(Kong et al., 2020) or metals, biopolymers (chitosan, alginate), layered double hydroxides (LDHs)(Tang, Qiu, Lu, & Shi, 2020), or biochar. As an example, magnetic graphene composites are made by the co-precipitation of iron salts onto GO or rGO sheets, which are easy to separate with the help of an external magnetic field (Melchor-Durán et al., 2024). On the same note, the synthesis of graphene-LDH composites is done by co-precipitation or hydrothermal, solvothermal, solgel methods which gives them a better adsorption capability due to synergetic effect.

Applications

1. Adsorption of Heavy Metals

The second-generation graphene-derived, such as graphene oxide (GO), reduced graphene oxide (rGO), heteroatom-doped graphene, and functionalized graphene-based nanocomposites have been developed as the effective adsorbents in the purification of toxic heavy metals in wastewater. Their outstanding physicochemical characteristics, such as, high specific surface area, tunable facades, and prolific oxygen-based functional groups allow their high level of interrelating with a vast variety of metal ions, including Pb (II), Cd (II), Cr (VI), Hg (II), and As (III/V).

The Graphene oxide in particular has a greater adsorption capacity owing to the availability of the hydroxyl, carboxyl and epoxide functions located over the basal plane as well as around the edges of the plate. These functional groups serve as active sites of attachment of metal ions, adsorption through coordination and electrostatic support. Although it has fewer oxygen functionalities, reduced graphene oxide also has better electrical conductivity and can be configured as a hybrid with metal oxides (e.g., Fe3O4, TiO2, MnO2) or as a hybrid with layered double hydroxides (LDHs), in order to enhance structural stability and reusability (Amrutha, Jeppu, Girish, Prabhu, & Mayer, 2023).

Besides, the substitution of the carbon in the graphite structure with heteroatoms, including nitrogen, sulfur, and phosphorus, creates more active sites and regulates electron density, which greatly increases the adsorption affinity with particular heavy metal ions. Sophisticated architectures have also been observed to be highly effective in realistic wastewater application systems because of their simple isolation and recycling of graphene-based materials on bio-inspired functionalized architectures that include three-dimensional graphene aerogels, magnetic graphene alloys, and bio-inspired functionalized graphene materials.

2. Mechanism of Adsorption

The synergistic mechanisms control the adsorption of heavy metals on graphene derivatives and all of them lead to substantial removal efficiency. Such mechanisms are electrostatic attraction, surface complexation, ion exchange, π-π interactions and precipitation.

The electrostatic interactions are predominant specifically in aqueous whereby the pH of the solution affects the surface charge of the graphene derivatives. When the functional groups of the negatively charged GO or doped graphene are at suitable pH, positively charged metal ions, including Pb2+ and Cd2+, are drawn to it (Elgengehi, El-Taher, Ibrahim, Desmarais, & El-Kelany, 2020). On the other hand, in the case of anionic species such as Cr (VI), the binding can be either through electrostatic attraction conditions of protonated surfaces or reduction to less toxic Cr (III), then adsorption.

Another important mechanism, surface complexation, is where the metal ions are coordinately bound to the oxygen and heteroatom functional groups present on the surface of the graphene. As an example, metal ions can be chelated by carboxyl and hydroxyl groups in which case they form stable inner-sphere complexes. In graphene which has been doped with heteroatoms, nitrogen functional groups serve as electron donors and increase binding affinity by coordination interactions.

The adsorption is also enabled by ion exchange which is especially good in graphene-based composites like in LDH/graphene hybrids, where anions between the layers can be replaced by metal ions or complexes of the metal. Also, redox reactions can take place, in particular, in systems where reduced graphene oxide is used or composite materials where toxic metal ions of the type Cr (VI) are reduced to less toxic oxidation states. The presence of all these mechanisms allows graphene derivatives to display highly versatile and strong adsorption properties in a wide range of environmental parameters.

3. Adsorption Efficiency

Graphene-based materials adsorption efficiency is generally determined based on the parameters of adsorption capacity (q81), removal percentage, kinetics, and models of isotherm. It has been reported that exceptionally high adsorption capacities of graphene derivatives have been incredibly high and sometimes surpass those of conventional adsorbents: activated carbon, zeolites and polymeric resins. As an illustration, graphene oxide-based materials have been shown to have adsorption capacities of Pb(II) and Cd(II) of more than 300–500 mg g -1, and has been functionally functionalized to give higher adsorption capacities under conditions of surface modification and experimental set-up.

The kinetics of adsorption in graphene systems are usually pseudo-second-order meaning that the chemisorption process is rate-limiting. The rate of rapid adsorption is usually caused by high accessibility of active sites and low diffusion resistance of two-dimensional structures. The Langmuir model is often consistent with isotherm experiments that imply monolayer adsorption by homogeneous surfaces but Freundlich behavior is also met in some cases in heterogeneous systems(Amrutha et al., 2023).

Environmental conditions like pH, temperature, ionic strength and competing ions are important factors that affect the performance of adsorption. The ideal PH values are usually in mildly acidic to neutral depending on the target metal ion and surface chemistry of the adsorbent used. Thermodynamic studies tend to demonstrate that the adsorption processes are spontaneous and endothermic which implies better operation at high temperature.

Notably, the next-generation derivatives of graphene have a high adsorption reusability and regeneration ability and retain the high adsorption efficiency after multiple cycles with a negligible reduction in efficiency. In some cases, the graphene composites which are magnetized have made the recovery process easy with the help of external magnetic fields, thus making its operational feasibility in large scale environments easier (Kong et al., 2021).

4. The Integrated Perspective on Practical Applications Has to be Integrated

Introduction of graphene-based derivatives to the treatment process of the waste water is a revolutionary technology of the environmental cleaning process. Their use is in batch adsorption systems applications, fixed-bed column, membrane filtration, and hybrid treatment. Graphene based adsorbents can also be applied in the detoxification of heavy metal in industrial environment wherein mining effluents, electroplating wastewater and battery manufacturing discharge have been successfully detoxified with a very high-performance and efficient scale.

Besides, the interaction of graphene derivatives and green synthetic strategies such as plant-mediated functionalization and bio-inspired composites is in line with the principles of sustainable engineering and green chemistry. This decreases environmental impact as well as improves biocompatibility and economy.

All in all, the next generation graphene variants are a highly useful and high-performance platform in the adsorption and detoxification of heavy metals, and have immense possibilities in practical use in more advanced wastewater treatment technologies (Schmidt, Dou, & Sydlik, 2023)

Challenges and Future Perspectives

1. Challenges

Although next-generation graphene derivatives have a tremendous potential in wastewater treatment, there are a number of scientific, technological and economic obstacles that prevent their large-scale application. The main shortcoming is the capability to produce high quality graphene-based materials in a scalable synthesis. The methods of chemical vapor deposition and modified Hummer’s method in most cases have a high energy consumption, toxic substances, and multi-step processing, which conflict with the principles of sustainable engineering. Also, the physicochemical properties, i.e. surface area, defect density, functional group distribution, etc. must be uniform, which is a long-standing story that can impact the adsorption performance and reproducibility.

The other important issue of concern is the stability and reusability of graphene derivatives in the actual environment. Organic pollutants, variation of pH, presence of competing ions and organic pollutants in heavily contaminated wastewater may significantly reduce the adsorption performance of the material. Graphene π-π stacking and van der Waals forces cause agglomeration of sheets to give a further decrease in the effective surface area and restricts the number of active adsorption sites. In addition, re-generating spent adsorbents without any structural damage is a technical bottleneck.

Special attention also should be paid to toxicological issues. Though the materials made of graphene are a very useful adsorbent, there is a lack of clear comprehension of their potential eco-toxicity and the consequences of using these materials on the environment in the long run. When nanoscale graphene particles are released into the aquatic life, it can be harmful to the microbial community and higher organisms, leading to the concern of biosafety and regulation.

Engineering wise, it is still difficult to be integrated with the existing wastewater treatment systems. Implementing the shift between the laboratory size batch adsorption research to the continuous flow type of the industrial systems presupposes highly sophisticated reactor construction, process optimization, and cost-effectiveness evaluation. Moreover, the absence of standardized guidelines on the performance assessment makes the comparisons and bench marking of various materials of graphene composite difficult (Faysal Hossain, Akther, & Zhou, 2020).

2. Future Outlook

The future of graphene derivative in heavy metal detoxification has a great potential due to technology improvement in nanotechnology, material science, and green chemistry. The development of industries and hybrid graphene-based nanocomposites, including graphene oxide (GO) and reduced graphene oxide (rGO) with metal oxides and polymers and bio-based materials, is one of the directions. Such hybrid systems are capable of improving selectivity, adsorption capacity and stability of structure by synergy.

The methods of green synthesis will have crucial roles to play in the issue of sustainability. The use of plant extract in the production of graphene derivatives, microbial routes, and biomass-derived carbon sources are in line with the principles of environmental friendliness and minimize the use of chemicals, which can cause hazards. These strategies reduce environmental impact as well as enhance biocompatibility and are therefore increased in suitability of applications in the real world.

The other trend is the use of graphene derivatives in the context of the membrane technology, as well as in the smart filtration systems. Graphene membranes have demonstrated high permeability, mechanical stability and pore structure that is tunable and therefore they are able to absorb heavy metal ions at low energy. The combination between the adsorption and the filtration process in a single platform has great benefits to deploy on industrial level.

Artificial intelligence and machine learning are also becoming popular in materials design and optimization of the process. The predictive modeling has the power to speed up the realization of new graphene-based adsorbents with specific characteristics and the real time monitoring can boost the performance of a wastewater treatment facility.

Moreover, investment in the future investigation based on the life cycle assessment (LCA) and techno-economic analysis should be targeted at assessing the environmental and economic viability of the graphene-based technologies. The regulations and safety rules are also required to be set in order to achieve the responsible development and implementation.

Conclusion

In summary the next-generation graphene derivatives constitute an exemplary category of materials have been used in the process of removing heavy metal in the wastewater with a high potential of adsorption, tunable surface chemistry, as well as multifunctional applications. Their capability to deal with the emergency environmental issues agrees with the sustainability of engineering and development of green technology. Nevertheless, there are a number of obstacles such as scalability, stability, possible toxicity, and integration into the system that have to be overcome systematically to be able to achieve their potentials.

The progress in the area of green synthesis, the hybrid design of materials, and the intelligent treatment is likely to overcome all the existing limitations and open the way to the practical implementation. There will be a need to have interdisciplinary synergies between materials scientists, environmental engineers, and policymakers in an effort to cast a bridge between laboratory research and industrial application. Conclusively, through everlasting innovation and sustainable development, the graphene-based technologies have a lot of potential as far as the realization of effective, sustainable, and affordable wastewater remedies is concerned in the nearest future.

References

1. Ain, Q. U., Farooq, M. U., & Jalees, M. I. (2020). Application of Magnetic Graphene Oxide for Water Purification: Heavy Metals Removal and Disinfection. Journal of Water Process Engineering, 33, 101044. https://doi.org/10.1016/J.JWPE.2019.101044
2. Amrutha, Jeppu, G., Girish, C. R., Prabhu, B., & Mayer, K. (2023). Multi-component Adsorption Isotherms: Review and Modeling Studies. Environmental Processes, 10. https://doi.org/10.1007/S40710-023-00631-0
3. Elgengehi, S. M., El-Taher, S., Ibrahim, M. A. A., Desmarais, J. K., & El-Kelany, K. E. (2020). Graphene and graphene oxide as adsorbents for cadmium and lead heavy metals: A theoretical investigation. Applied Surface Science, 507, 145038. https://doi.org/10.1016/J.APSUSC.2019.145038

4. Faysal Hossain, M. D., Akther, N., & Zhou, Y. (2020). Recent advancements in graphene adsorbents for wastewater treatment: Current status and challenges. Chinese Chemical Letters, 31(10), 2525–2538. https://doi.org/10.1016/j.cclet.2020.05.011
5. Kong, Q., Preis, S., Li, L., Luo, P., Wei, C., Li, Z., … Wei, C. (2020). Relations between metal ion characteristics and adsorption performance of graphene oxide: A comprehensive experimental and theoretical study. Separation and Purification Technology, 232, 115956. https://doi.org/10.1016/J.SEPPUR.2019.115956
6. Kong, Q., Shi, X., Ma, W., Zhang, F., Yu, T., Zhao, F., … Wei, C. (2021). Strategies to improve the adsorption properties of graphene-based adsorbent towards heavy metal ions and their compound pollutants: A review. Journal of Hazardous Materials, 415. https://doi.org/10.1016/j.jhazmat.2021.125690
7. Melchor-Durán, A. P., Moreno-Virgen, M. R., Bonilla-Petriciolet, A., Reynel-Ávila, H. E., Lucio Ortiz, E., & González-Vázquez, O. F. (2024). Heavy Metal Removal from Water Using Graphene Oxide in Magnetic-Assisted Adsorption Systems: Characterization, Adsorption Properties, and Modelling. Separations 2024, Vol. 11, 11(10). https://doi.org/10.3390/separations11100294
8. Mohammed, M. N., Aljibori, H. S. S., Jweeg, M. J., Al Oqaili, F., Abdullah, A., Abdullah, O. I., … Al-Azawi, K. (2024). A Comprehensive Review on Graphene Oxide Based Nanocomposites for Wastewater Treatment. Pol. J. Chem. Tech, 26(1). https://doi.org/10.2478/pjct-2024-0007
9. Sadeghi, M. H., Tofighy, M. A., & Mohammadi, T. (2020). One-dimensional graphene for efficient aqueous heavy metal adsorption: Rapid removal of arsenic and mercury ions by graphene oxide nanoribbons (GONRs). Chemosphere, 253, 126647. https://doi.org/10.1016/J.CHEMOSPHERE.2020.126647
10. Schmidt, S. J., Dou, W., & Sydlik, S. A. (2023). Regeneratable Graphene-Based Water Filters for Heavy Metal Removal at Home. ACS ES&T Water, 3(8), 2179–2185. https://doi.org/10.1021/acsestwater.3c00010
11. Tang, Z., Qiu, Z., Lu, S., & Shi, X. (2020). Self-assembling 2D/2D (MXene/LDH) materials achieve ultra-high adsorption of heavy metals Ni2+ through terminal group modification. Elsevier, 9(1), 800–819. https://doi.org/10.1515/NTREV-2020-0065/HTML
12. Viprya, P., Kumar, D., & Kowshik, S. (2023). Study of Different Properties of Graphene Oxide (GO) and Reduced Graphene Oxide (rGO). Engineering Proceedings 2023, Vol. 59, 59(1). https://doi.org/10.3390/ENGPROC2023059084

Frontiers in Chemical Science

ISBN: 978-93-49938-06-9| Year: 2026 | pp: 92 – 106 |

Solar Cell and Photovoltaic Chemistry Fundamentals of Dye-Sensitized Solar Cells: Working Principles and Kinetics

[1]Kanchana Venkatesan

[1]Dinesh Kumar

[2]Padmavathi. R

[1]Department of Chemistry, AMET University, Chennai, Tamilnadu

[2]Department of Chemistry, Vel tech Multi tech Dr. Rangarajan Dr. Sakunthala, Engineering college, Avadi, Chennai, Tamil Nadu.

Email: kanrishi04@gmail.com

Article DOI Link: https://zenodo.org/uploads/19637896

DOI: 10.5281/zenodo.19637896

Abstract

Dye-sensitized solar cells (DSSCs) constitute a novel and economical means of converting solar energy into electricity using a photo-electrochemical process. As opposed to other solar cells based on silicon technology, the dye molecules function as light absorbers which release electrons that pass into the semiconductor, usually titanium dioxide (TiO_2). The main components of the cell include the photo-anode, sensitized dye, electrolyte, and counter-electrode, whose interaction helps create optimal conditions for charge separation and transfer of electrons. The whole process takes place through a number of steps such as photon absorption, electron injection into the semiconductor, transfer of electrons through the semiconductor lattice, dye molecule regeneration, and reduction and oxidation reactions of the electrolyte. The efficiency of operation of DSSC highly depends on the electron transfer process and charge transfer kinetics in DSSC. There have been recent advancements aimed at enhancing the efficiency of these solar cells by optimizing the performance of sensitizing dyes, semiconductor materials, electrolytes, and counter electrodes.

Keywords: Titanium dioxide (TiO_2); Sensitizing dye; Electron transfer mechanism; Charge transfer kinetics; Renewable energy; Photo electrochemical process; Nanostructured semiconductors; Solar energy conversion.

Introduction

The world energy demand has increased very fast and the scarcity of conventional fossil fuel sources has fueled the quest to find renewable sources of energy and clean energy. Scientists are currently developing renewable energy sources like solar, wind, hydro and geothermal energy to satisfy the energy requirements in the future. Solar energy is one of these options that are said to have the greatest potential due to its abundance, cleanliness and are common throughout the world. Photovoltaic (PV) technologies directly transform sunlight directly into electrical energy and have become an important element in the world renewable energy infrastructure. The conventional silicon-based solar cells are very much prevalent in the commercial market because of their relatively high-power conversion efficiency (PCE) and stability. But the manufacture of silicon solar cells involves high-purity of materials, complicated manufacturing process and high temperature which contribute readily to the cost of production. These shortcomings have encouraged the exploration of alternative photovoltaic technologies which are economical, versatile and less cumbersome to manufacture. The new technologies are thin-film solar cells, organic solar cells, perovskite solar cells, and dye-sensitized solar cells (DSSCs). Of these, DSSCs have received a lot of interest because of their exclusive operating principle, low-cost production and the capacity to work under diffuse light conditions. DSSCs are now the third generation of photovoltaic devices and were inspired by natural photosynthesis, light absorbing pigments absorb solar energy, which is then converted to chemical energy.

Equally, and in the same case, the dye molecules in DSSCs serve as photosensitizers that capture sunlight and trigger the mechanisms of electron transfers to produce electrical energy. The use of DSSCs was initially invented by Brian O’Regan and Michael Gratzel in 1991, which proved a significant breakthrough in solar cell research. Their article has shown that nanostructured titanium dioxide ($TiO2$) can be used with light-absorbing dyes to create efficient solar cells, also known as Gratzel cells. The nanocrystalline $TiO2$ is found to enhance the surface area of dye adsorption which boosts light collection and electron injection. A standard DSSC comprises of a photoanode, sensitizer dye, an electrolyte, and counter electrode. Dye molecules capture sunlight and add electrons into the conduction band of $TiO2$. The electrons are then directed through the semiconductor to the external circuit to produce electricity. The redox electrolyte provides electrons that re-oxidize the oxidized dye molecules thus completing the electrochemical cycle. The fact that DSSCs can be effectively utilized in low light or diffuse-light environments (indoor or on cloudy days) is one of the merits of the technology, enabling it to find application in portable electronics or building-integrated photovoltaics (BIPV). Fabrication is not very difficult, and low-cost materials and techniques include screen printing and low-temperature deposition. Recent developments are aimed at enhancing the efficiency and stability of DSSCs through the preparation of superior dyes, alteration of semiconductor nanostructures, optimization of electrolytes and alternative counter electrode materials. The comprehensive knowledge on how to transfer electrons and charge kinetics are necessary when it comes to enhancing performance and creating next-generation equipment.

Overview of Dye-Sensitized Solar Cells

Dye-sensitized solar cells (DSSCs) are a type of photovoltaic cells that produce electrical energy by a photoelectrochemical reaction to solar energy. DSSCs also utilize a photosensitive dye to absorb the light and produce electrons, unlike traditional semiconductor solar cells that use a p-n junction to separate charge carriers. In this method, it is easier to fabricate, and the materials are cheaper, but the energy conversion efficiency is moderate. Brian O'Regan and Michael Grätzel were the first to establish the idea of DSSCs, described in 1991 as an efficient solar cell made with an efficient titanium dioxide ($TiO2$) nanocrystallite coated with a ruthenium-based dye. As a result of this groundbreaking work, DSSCs can be called Grätzel cells. Their invention brought a new method of converting solar energy through nanostructured semiconductor materials and molecular sensitizers, which has since captured a lot of interest in materials science, electrochemistry, nanotechnology, and renewable energy studies [2,4].

A standard DSSC is composed of four main parts, namely, a photoanode, a sensitizer dye, an electrolyte, and a counter electrode, mounted between two conductive substrates. The photoanode, typically a nanostructured film of TiO 2 on a transparent conductive surface like fluorine-doped tin oxide (FTO), offers a great surface area to adsorb dye, increasing light absorption. The sensitizer dye absorbs photons and is electronically excited injecting electrons into the conduction band of TiO 2, a process that takes place within the femtosecond to picosecond time scale, which is efficient in charge separation. The injected electrons move through the interconnected TiO 2 net to the external circuit and generate electrical current. At the same time, oxidized dye molecules are re-reduced by a redox electrolyte, usually the iodide/triiodide (I -/I 3 -) couple, which keeps charge neutrality in the device. The reduction of triiodide ions back to iodide occurs on the counter electrode which is usually coated with platinum or some other catalyst material thereby completing the electrochemical cycle [5]. DSSCs are able to work efficiently in low-light and diffuse conditions, e.g. indoor or cloudy, so they can be used in portable electronics, indoor energy harvesting, smart sensors, and building-integrated photovoltaic systems [6]. Moreover, they are made using cheap materials and low temperature processing methods, including screen printing or blade coating which renders mass production economically viable. DSSCs are also mechanically flexible, tuneable to colours and transparent, allowing it to be incorporated into windows and building facades to combine aesthetics and functional energy production. Notwithstanding these benefits, DSSCs have shortcomings such as reduced long-term stability, leakage of electrolyte, and reduced efficiency than crystalline silicon solar cells. The existing studies are aimed at improving stability, the creation of solid-state electrolytes, and the creation of improved sensitizing dyes to boost performance. As the materials science and nanotechnology continue to develop, DSSCs will become a larger part of the future renewable energy systems.

Solar Cell Components: Dye-Sensitized Solar Cells

A dye-sensitized solar cell (DSSC) is an interconnected system that operates together to transform solar energy into electrical energy. A photoanode, a sensitizer (dye), an electrolyte and a counter electrode are the primary constituents of a DSSC. Each part is involved in a particular part of the photovoltaic mechanism and the working efficiency of the device highly relies on the characteristics of the materials and their interactions. DSSCs design is founded on the effective light absorption, rapid electron injection, effective charge transfer, and low recombination losses. To achieve optimal performance of the devices, it is important to know the structure and the work of each component.

1. Photoanode

The photoanode is an electrode collection of electrons and a surface where dyes are adsorbed. It consists usually of a nanostructured semiconductor, most often titanium dioxide (TiO 2), applied onto a transparent conductive substrate (such as fluorine-doped tin oxide (FTO) glass). Titanium dioxide is a popular material because it has a high level of chemical stability, non-toxicity, low cost, and appropriate electronic characteristics. The bandgap of TiO 2 is around 3.2eV, which means that it can be used as an efficient electron transport material, and it is transparent to visible light, so the sunlight can go through and strike the adsorbed dye molecules.

TiO2 is commonly produced in the form of nanoparticles in DSSCs, with a very porous structure. This nanostructure offers a very large surface area upon which dye can be adsorbed, and this can be many times greater than the geometric area of the electrode. The increased surface area means more dye molecules can be attached to the semiconductor, enhancing the amount of light absorbed and the overall cell efficiency [7]. TiO2 layer is usually deposited on the FTO substrates by screen printing, blade coating, spin coating, or spray pyrolysis. The film is then sintered at high temperature after deposition to improve the connectivity of particles and electron transfer. Photoanodes of other semiconductors studied include zinc oxide (ZnO), tin oxide (SnO2), and niobium oxide (Nb2O5), although TiO2 has been used most commonly because of its stability and compatibility with dyes. The electron transfer and recombination losses have been addressed by using modifications like metal ion doping, the addition of carbon nanomaterials and hierarchical nanostructure design.

2. Sensitizer (Dye)

The sensitizer or dye takes in sunlight and triggers the photoelectric process. Photons are absorbed by dye molecules, which cause electrons in the highest occupied molecular orbital (HOMO) to be excited to the lowest unoccupied molecular orbital (LUMO). These excited electrons are introduced into the conduction band of the semiconductor, which is usually TiO 2, within the femto seconds to picoseconds, which guarantees effective separation of charge and low energy loss.

A perfect dye must have:

- Good uptake in the visible spectrum.
- Large molar extinction coefficient.
- Efficient injection of the electron into the semiconductor.
- High chemical adsorption to the semiconductor surface.
- Long-term photochemical stability

Common Dyes Include

Ruthenium-based dyes: Ruthenium complexes are highly visible range absorbing and photochemically stable complexes. One of the most famous examples is N3 dye, which is commonly used in research in DSSC due to its efficiency and durability [8].

Organic Dyes

Metal-free organic dyes have low cost, large absorption coefficients and molecular structures that can be tuned. It is possible to design functional groups that improve light absorption and electron transfer.

Natural Dyes

Natural dyes are extracted plants, fruits, and flowers; they include anthocyanins, chlorophyll, and betalains and are eco-friendly alternatives. They tend to be less efficient compared to synthetic dyes, non-toxic, easily obtained, and sustainable [9].
Recently, the attention is paid to porphyrin-based dyes, co-sensitization techniques, and dyes that do not contain any metal to enhance the light harvesting and work of the device.

3. Electrolyte

The electrolyte facilitates the transfer of charges and restores the oxidized dye molecules upon the injection of electrons into the semiconductor. Majority of DSSCs utilize a redox couple, usually iodide/triiodide (I3-/I-). The oxidized dye is donated electrons by iodide ions which helps in the regeneration of the dye to enable it to absorb photons repeatedly.

The regeneration reaction is:

$$D+ + 2I^- \rightarrow D + I2$$

The resulting triiodide ions (I_3^-) are reduced to iodide at the counter electrode to keep the redox cycle going.

Electrolytes may be categorized as:

- Liquid electrolytes
- Solid-state electrolytes
- Gel electrolytes

Liquid electrolytes have high ionic conductivity but have leakage and evaporation problems. Solid-state and polymer gel electrolytes enhance stability and decrease leakage, and spiro-OMeTAD is a widely used material [10].

4. Counter Electrode

The cathode, which serves as the counter electrode, provides the completion of the electrical circuit by carrying electrons out of the external circuit to the electrolyte to allow the reduction of the triiodide ions:

$$I_3^- + 2e^- \rightarrow 3I^-$$

Traditionally, platinum on conductive glass (FTO) is selected because it is a good catalyst, conductive and stable to chemical reactions. Platinum is however, costly and alternatives have been investigated like:

- Carbon materials (carbon black, carbon nanotubes, graphite)
- Graphene-based materials
- Conductive polymers
- Transition metal compounds (cobalt sulfide, nickel sulfide)

The platinum performance is similar to that of carbon-based materials which are cost-effective and environmentally friendly. One of the major directions in the research on DSSC is the development of low-cost and efficient counter electrodes [11].

Principle of Dye-Sensitized Solar Cells

The principle of the functioning of the dye-sensitized solar cells (DSSC) is a photoelectrochemical process whereby sunlight is transformed into electrical energy through a number of electron transfer reactions. As opposed to the old-fashioned photovoltaic devices functioning on the principles of semiconductor p-n junction, the DSSC modules utilize a light-absorbing sensitizing dye molecule to produce excited electrons that are then injected into a semiconductor substance. The working of DSSCs resembles the natural photosynthesis process, whereby some light energy is trapped by pigments and transformed into chemical energy.

A standard DSSC comprises of a semiconductor nanostructured photoanode, which is coated with dye molecules, an electrolyte that contains a redox couple, and a catalytic counter electrode. As sunlight enters the device it undergoes a series of electrochemical reactions that result in the generation of electrical energy. Stepped processes that can be used to describe the overall functioning of DSSCs are light absorption, electron injection, electron transport, dye regeneration and electrolyte regeneration.

1. Light Absorption

Light absorption by the sensitizer dye molecules is the first step in working of DSSCs. The dye molecules are attached to the surface of the semiconductor material, most of the time titanium dioxide (TiO 2). On exposure to sunlight photons, the dye molecules absorb energy and get excited.
This formula can be expressed as:

$$D + h\nu \rightarrow D^*$$

Where D represents the dye molecule in the ground state, h the incident photon and D the excited state of the dye molecule.

2. Electron Injection

Upon excitation, the dye molecule transfers an electron to the conduction band of the semiconductor. The excited dye molecules release electrons very quickly to the conduction band of TiO2.
This can be put across as:

$$D^* \rightarrow D^+ + e^- (TiO_2)$$

The dye is oxidized (D+) and the injected electron is taken into the conduction band of TiO 2. This is usually done at a timescale of femtosecond up to picosecond, which guarantees effective charge separation.

3. Electron Transport

Once injected into the conduction band, the electrons flow through the nanostructured TiO 2 network to the transparent conducting electrode. The transport is primarily via diffusion via interconnected nanoparticles.
Effective electron transport requires:

- Semiconductor morphology
- Particle connectivity
- Crystallinity
- Reduction in trapping and recombination.

4. External Circuit Flow

When the electrons arrive at the transparent conducting substrate (e.g., FTO), they move through the external circuit producing electrical current. The electrons go through the load and arrive at the counter electrode.

5. Dye Regeneration

The dye is oxidized (D+) during the process of electron injection and needs to be regenerated. This takes place through the donation of electrons by iodide ions in the electrolyte.

$2D^+ + 3I^- \rightarrow 2D + I_3^-$

This regeneration should be rapid in order to avoid the recombination between electrons and oxidized dye.

6. Electrolyte Regeneration

It involves reducing the oxidized electrolyte species (I3-) at the counter electrode by electrons of the external circuit:

$I_3^- + 2e^- \rightarrow 3I^-$

Platinum or carbon-based catalysts are the materials that catalyze this reaction.

7. The Overall Photoelectric Cycle

The entire DSSC cycle consists of a cyclic process of
- Light absorption
- Electron injection
- Electron transport
- Dye regeneration
- Electrolyte regeneration

DSSCs are efficient depending on
- Good light absorption by the dye.
- Fast electron injection
- Efficient electron transport
- Rapid dye regeneration
- Suppression of recombination mechanisms.

Electron Transfer Mechanism

The electron transfer mechanism in DSSCs defines the efficiency of the conversion of the absorbed light to electrical energy [12-14].It takes place by exciting dye molecules, injecting electrons into the semiconductor, and transporting them across the semiconductor network, as well as potential recombination routes. Upon absorption of photons by dye molecules, electrons are excited out of the ground state into an excited state:

$D + h\nu \rightarrow D^*$

The excited dye injects an electron to the conduction band of TiO 2:

$D^* \rightarrow D^+ + e^- (TiO_2)$

This is a very fast process (femtoseconds -picoseconds), necessary to outcompete recombination.

Electron Transport

Diffusion is the process through which electrons pass through the TiO 2 network, between nanoparticles. The effectiveness is determined by:

- Particle connectivity
- Trap states
- Crystallinity
- Film thickness

Recombination Processes

Recombination decreases the efficiency of the device and takes place through two primary mechanisms:
Electron recombination with oxidized dye:

$e^- (TiO_2) + D^+ \rightarrow D$

Electron recombination with triiodide ions:

$e^- (TiO_2) + I_3^- \rightarrow I^-$

Energy Level Alignment

For efficient operation:

- The excited state of the dye should be higher than the conduction band of TiO2.
- The oxidation potential of electrolyte should be less than that of dye.
- This guarantees effective dye regeneration and electron injection.

Charge Transfer Kinetics

Charge transfer kinetics and recombination processes in the dye-sensitized solar cells (DSSCs) device have a significant effect on the performance and efficiency of the cells. Photoelectric conversion in DSSCs is a series of reactions of charge transfer, which should be fast and efficient to produce electrical energy [15]. These processes depend on the speed of converting absorbed solar energy to electrical energy which is the determinant of the efficiency of the conversion process. Therefore, to optimize the performance of DSSC, it is necessary to learn more about the kinetic characteristics of electron injection, electron transfer, recombination, and dye regeneration.
The main kinetic processes involved in DSSCs are:

- Electron injection of the excited dye molecule into the semiconductor.
- Electron transfer in the semiconductor network.
- Recombination of electrons with oxidized species in the electrolyte.
- The oxidized dye molecules were regenerated with the help of electrolyte.

- All these processes are important in determining the overall solar cell efficiency.
- Electron injection kinetics

1. Electron Injection with an Electrode

The first and one of the fastest processes in DSSCs is electron injection of an excited dye molecule into the conduction band of the semiconductor. Electrons: This is because when a photon is absorbed by a dye molecule, the electron is excited out of its ground state to higher energy level. The excited electron then moves into the conduction band of the semiconductor, which is usually titanium dioxide (TiO2). The electron injection mechanism is extremely fast, usually on the femtosecond to picosecond scale, and allows a high degree of charge separation and reduces recombination losses. [16-17]. Rapid electron injection is necessary since it is required to give the excited electron to the semiconductor before it gets lost to relaxation mechanisms.

The rate of electron injection is determined by various parts which include:

- Reference to Energy level alignment between the dye and the semiconductor.
- The character of anchoring groups in the dye molecule.
- Surface structure of the semiconductor.
- The intensity of the electronic interaction between the dye and the semiconductor.

2. Electron Transport in the Semiconductor

The electrons need to be conducted to the transparent conducting electrode after being injected electronically through the nanostructured network of semiconductor structures. The semiconductor layer of DSSCs is made of interconnected nanoparticles which create porous structure through which the electrons can flow through the substance. The electron movement in TiO2 is mostly by diffusion process where electrons flow by jumping between adjacent nanoparticles. The rate of electron transfer depends on the size of the particles, their crystallinity, trap states and the conductivity of the semiconductor material. Electron transfer needs to be efficient so that the electrons can arrive to the collection electrode prior to recombination taking place. The electron mobility can be improved by enhancing the semiconductor structure (i.e., nanowires, nanotubes, hierarchical nanostructures, etc.) [18]. It is possible to reduce the charge transfer resistance, which will improve the electron mobility.

3. Recombination Processes

Recombination is one of the main factors that reduce the efficiency of DSSCs. The process in which electrons in the semiconductor conduction band interact with oxidized species rather than move through the external circuit is called recombination.

The recombination pathways in DSSCs are two:

- Recombination of electrons in the semiconductor and oxidized dye molecules.
- Electron recombination with oxidized electrolyte species like triiodide ions(I3-).

Of these, in DSSCs, the most common loss mechanism is usually recombination with triiodide ions. The recombination processes decrease the number of electrons that produce the electric current and thus the power conversion efficiency of the device is reduced. Some of the strategies that the researchers have devised to minimize recombination losses include:

Surface passivation of the semiconductor.

- Blocking layers.
- Electrolyte composition optimization.
- Innovation of sophisticated sensitizing dyes.

It is also necessary to reduce recombination to enhance the open-circuit voltage and efficiency of DSSCs.

4. Dye Regeneration Kinetics

The regeneration of oxidized dye molecules has been another significant kinetic process in DSSCs. Once the electrons have been emitted, the dye is oxidized and must be replenished to a ground state so that it can again absorb photons. This regeneration occurs by a redox reaction between the oxidized dye and the electrolyte. In the majority of DSSCs the iodide/triiodide redox pair is employed in which iodide ions release electrons to the oxidized dye molecules.

The reaction describing the regeneration process may be presented as:

$2D^+ + 3I^- \rightarrow 2D + I_3^-$

This reaction should be fast to avoid the recombination of electrons in the semiconductor and oxidized dye molecules. Quick regeneration of dyes makes the solar cell operational continuously and keeps it highly efficient in photovoltaic production.

5. Methods of Charge Transfer Kinetics

A number of experimental methods are employed to examine the kinetic behavior of charge transfer processes in DSSCs. These methods assist researchers in the dynamics of the electron transfer and what factors constrain the performance of a device.

The most frequently employed methods are:

- Electrochemical Impedance Spectroscopy (EIS): to examine charge transfer resistance and recombination within the cell.
- Transient photocurrent and photovoltage measurements: to estimate the electron lifetime and recombination rates.

- Intensity Modulated Photocurrent Spectroscopy (IMPS): applied in the study of kinetics of electron transport.
- Intensity Modulated Photovoltage Spectroscopy (IMVS): applied to study recombination dynamics.

These methods give useful data concerning the charge transfer processes and the kinetic constraints of the DSSCs which enable researchers to develop more efficient photovoltaic systems.

Factors that affect the effectiveness of DSSCs

The performance and power conversion efficiency of dye-sensitized solar cells (DSSCs) are affected by physical, chemical, and environmental factors. The performance of DSSCs is determined by the effectiveness with which the device absorbs solar radiation, creates charge carriers, transfers electrons and reduces losses due to recombination. In this way, it is necessary to optimize these factors in order to enhance performance and long-term stability. The nature of the sensitizing dye and light-absorbing properties is one of the most significant influencing factors of DSSC performance. The dye molecule is a light-harvesting molecule and its capacity to absorb a large portion of the solar spectrum has a direct impact on energy conversion efficiency. The shape of the semiconductor material, which is usually TiO 2, is another significant aspect. Nanostructure with a high porosity has a high surface area to be used in the adsorption of dye, enhancing the absorption of light and the generation of charge. The composition of the electrolytes is also crucial. Ionic conductivity, viscosity and stability of the electrolyte influence charge transfer rates and performance of the device. DSSC efficiency is also affected by environmental conditions like temperature and light intensity. DSSCs also work well in low-light conditions and thus are applicable in indoor environments. Lastly, efficiency is greatly influenced by the recombination processes. To obtain high performance it is necessary to reduce recombination by means of better materials and design of the device.

Applications of Dye-Sensitized Solar Cells

DSSCs are of great interest due to their relatively low production cost, as well as due to its versatility and uncharacteristic operation. Unlike the conventional silicon-based photovoltaic cameras, DSSCs are effective even under low light conditions and diffused light implying that they are especially effective in a broad array of new applications. DSSCs can be produced on flexible substrates, and can be produced in other colors and in various levels of transparency, which would be appealing as technology and architecture. Among the potential uses of DSSCs is building-integrated photovoltaics (BIPV) [19]. This method involves the integration of solar panels into the building materials including windows, facades and roof constructions. DSSCs are especially applicable in this application since they can be produced as semi-transparent or colored solar cells that can be used to transmit natural light through and produce electricity. This twofold purpose enables the buildings to produce renewable energy without affecting the architectural elegance of the buildings.

The other significant use of DSSCs is in handheld electronics. DSSC modules are lightweight, flexible, and easily operable in the conditions of indoor lighting, which makes them suitable to power small electronics like mobile phones, sensors, calculators, and wearable electronics. They are highly applicable in the indoor generation of electricity as they can utilize the artificial sources of light to generate electricity. Indoor energy harvesting systems also display good prospects of DSSCs. A variety of modern electronics, such as wireless sensors, Internet of Things (IoT) devices and smart home systems, need energy sources with low power which are able to work even in the ambient light. DSSCs have already demonstrated great performance with regard to fluorescent and LED lighting and thus it has a potential solution to the same. The other innovative use is the creation of the transparent or semi-transparent solar cells of windows. These solar cells would be incorporated in window glass which will enable buildings to produce electricity without obscuring the view and natural light. This method is especially applicable in the contemporary urban architecture, where the energy saving design is vital. Besides, DSSCs may be applied in wearable electronics, smart fabrics, and flexible energy devices. Their mechanical flexibility enables them to be incorporated in fabrics or curved surfaces, and make portable energy generation systems. DSSCs can also be used as decorative architectural devices due to the color tunability and aesthetic appearance of the device. DSSCs may be prepared in a variety of colors by choosing other dyes and incorporated into structures that are attractive to the eye [20]. In general, DSSCs are quite an appropriate type of devices due to the peculiarities of their cost, flexibility, transparency, and the possibility to work in low-light conditions, which makes them extremely applicable in numerous practical applications.

Future Perspectives

Dye-sensitized solar cells (DSSCs) have become a promising photovoltaic technology because they are cheap to manufacture, are easily prepared and can perform efficiently in low-light conditions. These problems are long-term stability problems, leakage of electrolytes, relatively low efficiency in comparison with silicon based solar cells and degradation of materials with time. A key area of research is the realization of solid-state electrolytes instead of liquid electrolytes. High ionic conductivity is offered by liquid electrolytes which have a problem of leakages, evaporations and stability. Gel and solid-state electrolytes are more stable and durable, and are considered to be attractive to next generation DSSCs. The other significant field of study is the production of superior sensitizing dyes. New organic dyes, metal free dyes, porphyrin-based sensitizers with wider absorption spectrums and high light harvesting properties are being investigated. The application of co-sensitization strategies with various dyes is also under investigation in order to increase efficiency.

Nanotechnology developments are also helping in enhancing DSSC performance. Nanostructured forms of semiconductor materials, including TiO 2 nanotubes, nanowires, and hierarchical forms are found to offer improved electron transport mechanisms and minimized recombination losses. It has also demonstrated good results with the addition of carbon-based materials, graphene and quantum dots. Secondly, there is a study on developing inexpensive substitutes to platinum counter electrodes. As possible substitutes, materials like carbon nanotubes, graphene, conductive polymers, and transition metal compounds are under investigation. As further advances are made in materials science and in the engineering of devices, DSSCs will have an even greater role in renewable energy systems of the future, especially in building-integrated photovoltaics, wearable electronics, and energy harvesting within the interior.

Conclusion

Dye-sensitized solar cells (DSSCs) are a new and promising photovoltaic technology. As opposed to silicon based solar cells, DSSCs work based on a photoelectrochemical process whereby dye molecules absorb sunlight and cause excited electrons to move onto a semiconductor material. This special working principle ensures that DSSCs can be produced with relatively cheap materials and less complicated processing methods, and hence are an economical substitute to solar energy conversion. DSSCs have a number of benefits such as flexibility, transparency, and high performance at low-light conditions, which have rendered them applicable to the current energy applications. The mechanism of DSSCs is that light is absorbed, electrons are injected, transported and the dye and electrolyte regenerated. Charge transfer kinetics and recombination behaviour are highly dependent on the efficiency of these processes.

The chapter has addressed the basic properties of DSSCs such as its structure, working principle, electron transfer and charge transfer kinetics. The functions of the main products including photoanode, sensitizing dye, electrolyte and counter electrode have been mentioned. Issues affecting the performance of the devices such as semiconductor morphology, dye properties, composition of electrolytes and process of recombination have also been discussed. Despite the great achievements of DSSCs, there are still problems like long-term stability, the enhancement of efficiency, and the optimization of materials. Further study in materials science and nanotechnology should overcome these problems and improve the work of DSSC.

All in all, DSSCs possess high potential as renewable energy technology, which is sustainable and environmentally friendly. These will have a role to play in future photovoltaic systems with further development, particularly in building-integrated photovoltaics, portable electronics, and indoor energy harvesting.

References

1. Dragonetti, C., et al. (2021). Recent advances in dye-sensitized solar cells. Molecules, 26(9), 2461.
2. Muñoz-García, A. B., et al. (2021). Dye-sensitized solar cells strike back. Chemical Society Reviews, 50, 12450–12550.
3. Rahman, S., et al. (2023). Research on dye-sensitized solar cells: dyes and device performance. RSC Advances, 13, 10000–10020.
4. Korir, B. K., et al. (2024). A review on the current status of dye-sensitized solar cells toward sustainable energy. Energy Science & Engineering.
5. Saud, P. S., et al. (2024). Dye-sensitized solar cells: fundamentals, recent progress and future prospects. Solar Energy Materials and Solar Cells.
6. Iman, R. N., et al. (2024). Advancements and optimization strategies in dye-sensitized solar cells: components, stability and efficiency enhancement. Inorganic Chemistry Communications.
7. Malhotra, S. S., et al. (2024). Metal-free and natural dye-sensitized solar cells: progress and perspectives. Sustainable Energy & Fuels.
8. Barichello, J., et al. (2024). Bifacial dye-sensitized solar cells for indoor and outdoor applications. Journal of Materials Chemistry C.
9. Vallejo, W., et al. (2024). Meta-analysis of sensitizers used in dye-sensitized solar cells. Nanomaterials.
10. Dhorkule, M., et al. (2024). Efficiency evaluation of dye-sensitized solar cells using natural pigments. EcoMat.
11. Pirdaus, N. A., et al. (2024). Fungal pigments as natural dyes for dye-sensitized solar cells. SN Applied Sciences.
12. Saud, P. S., et al. (2024). Working mechanism and material innovations in DSSCs. Solar Energy Materials and Solar Cells.
13. Ávila, M., et al. (2025). Thermodynamic and kinetic considerations in dye-sensitized solar cells. Frontiers in Coatings and Interface Engineering.
14. Najihah, M. Z., et al. (2025). Enhanced efficiency of dye-sensitized solar cells using polyaniline-decorated electrodes. Ceramics International.
15. Marsya, M. A., et al. (2025). Highly transparent dye-sensitized solar cells with UV-absorbing dyes. Scientific Reports.
16. Koswatta, A. P., et al. (2025). Boosting DSSC efficiency using carbon quantum dots. ACS Omega.
17. Hasan, M. M., et al. (2025). Computational design of metal-free porphyrin dyes for DSSCs. Energy Informatics.
18. Nurfani, E., et al. (2025). Natural dye combinations for improved DSSC performance. Energy Materials Research.
19. Iman, R. N., et al. (2024). Optimization strategies for improving DSSC stability and efficiency. Inorganic Chemistry Communications.

ABOUT THE EDITORS

Dr. Arun Karansing Valvi

He is an Assistant Professor in the Department of Chemistry at Rayat Shikshan Sanstha's Annasaheb Awate College, Manchar holding a Ph.D. from ICT Mumbai (2019) and an M.Sc., with specialization in Organic Chemistry from KBCNMU, Jalgaon (2013). He has over 6 years of teaching experience at undergraduate and postgraduate levels and 12 years of research experience. His academic contributions include 13 research publications, 1 patent, 3 books, and 5 book chapters. He is actively involved in research, with one ongoing ASPIRE Research Mentorship Grant project under SPPU, Pune and one completed project. Dr. Valvi is a recognized Research Supervisor at Savitribai Phule Pune University (2023–2050) and served as a reviewer for the journal Materials Today: Proceedings (Elsevier). He has participated in multiple professional development activities, including two refresher courses, one orientation programme, ten faculty development programmes, and one short-term course.

Mr. Anand Kumar Mishra

He is currently pursuing his Ph.D. on catalytic treatment for removal of environmentally unfriendly metals from industrial waste water at Deen Dayal Upadhyay Gorakhpur University, Gorakhpur, India. He completed his M.Sc. in Chemistry in 2021 from M.L.K. P.G. College, Balrampur, affiliated with Siddhartha University, Uttar Pradesh, and holds a B.Ed. degree completed in 2023. His academic journey reflects his commitment to both chemistry and education. He has contributed five book chapters published by Bhumi Publishing, India. showcasing his growing research potential. Additionally, he has served as an editor for three books published by national and international publications . His areas of interest include catalysis and its diverse applications in chemical sciences. Mr. Mishra continues to focus on advancing his research skills and knowledge in chemistry, aiming to contribute significantly to the field through quality publications and academic initiatives in the coming years.

Dr. M. Velammal

She is an experienced academician in the field of Chemistry with over 24 years of teaching experience at Yadava College, Madurai, where she serves as an Assistant Professor. Currently working as Assistant Professor at NPR College of Engineering and Technology. She completed her Ph.D. in Chemistry in 2021 from Thiagarajar College, affiliated with Madurai Kamaraj University, with research focused on oxidation studies of dipeptides and nucleobases. She holds an M.Phil. (2001), M.Sc. (1998), and B.Sc. (1995) in Chemistry, all with First Class distinction. Her research contributions include multiple publications in reputed national and international journals, covering areas such as polymer chemistry, medicinal plants, antioxidants, and nanocomposites. She has actively participated in numerous national and international conferences, presenting research papers and engaging in faculty development programs, workshops, and webinars. Additionally, she has contributed to academic literature through book publications and has been involved in interdisciplinary research related to medicinal chemistry and environmental applications.

Dr. Swati Dattatray Burungale

She is an Associate Professor Delonix Society's Baramati College of Pharmacy, Barhanpur, Baramati. She has over 13+ years of teaching experience at the undergraduate level in the field of pharmaceutical sciences. She has demonstrated consistent commitment to academic excellence, student development and subject expertise. She holds a Ph.D. in Pharmacy (2024) from Mansarovar Global University, Bhopal, with a strong research orientation. Dr. Burungale possesses strong teaching competencies across core pharmaceutical subjects, including: Pharmaceutical Inorganic Chemistry Pharmaceutical Organic Chemistry Medicinal Chemistry Pharmaceutical Analysis Her teaching approach focuses on conceptual clarity, practical application and student-centric learning methodologies. She is an active member of the Association of Pharmaceutical Teachers of India (APTI) and has continuously contributed to professional development by participating in 50+ conferences, Faculty Development Programs (FDPs), workshops and Short-Term Training Programs (STTPs). With a blend of academic rigor and practical insight, Dr. Burungale continues to contribute significantly to pharmaceutical education and research.

Nature Light Publications

309 West 11, Manjari VSI Road, Manjari Bk.,
Haveli, Pune- 412 307.
Website: www.naturelightpublications.com
Email: naturelightpublications@gmail.com
Contact No: +919822489040 / 9922489040

Nature- 95

ISBN: 978-93-49938-06-9
9 789349 938069
Price- 720/-