GOVERNMENT DEGREE COLLEGE FOR WOMEN (A)

Ramagiri • Nalgonda • Telangana

TWO-DAY INTERNATIONAL SEMINAR

CHEMISTRY

PROCEEDINGS

SPECIAL ISSUE – FULL LENGTH ARTICLES FROM INTERNATIONAL SEMINAR

"New Vistas of Chemistry – An Interdisciplinary Approach"



Organized by

Department of Chemistry

Government Degree College for Women

Ramagiri • Nalgonda – Telangana, India

7 – 8 January 2026

ISSN: 3066-0637
February - 2026
Volume-III Issue-I (I)

Editor
Dr. Babalola, Ayodele Samuel

INTERNATIONAL JOURNAL OF RESEARCH STUDIES ON ENVIRONMENT, EARTH, AND ALLIED SCIENCES (*IJRSEAS*)

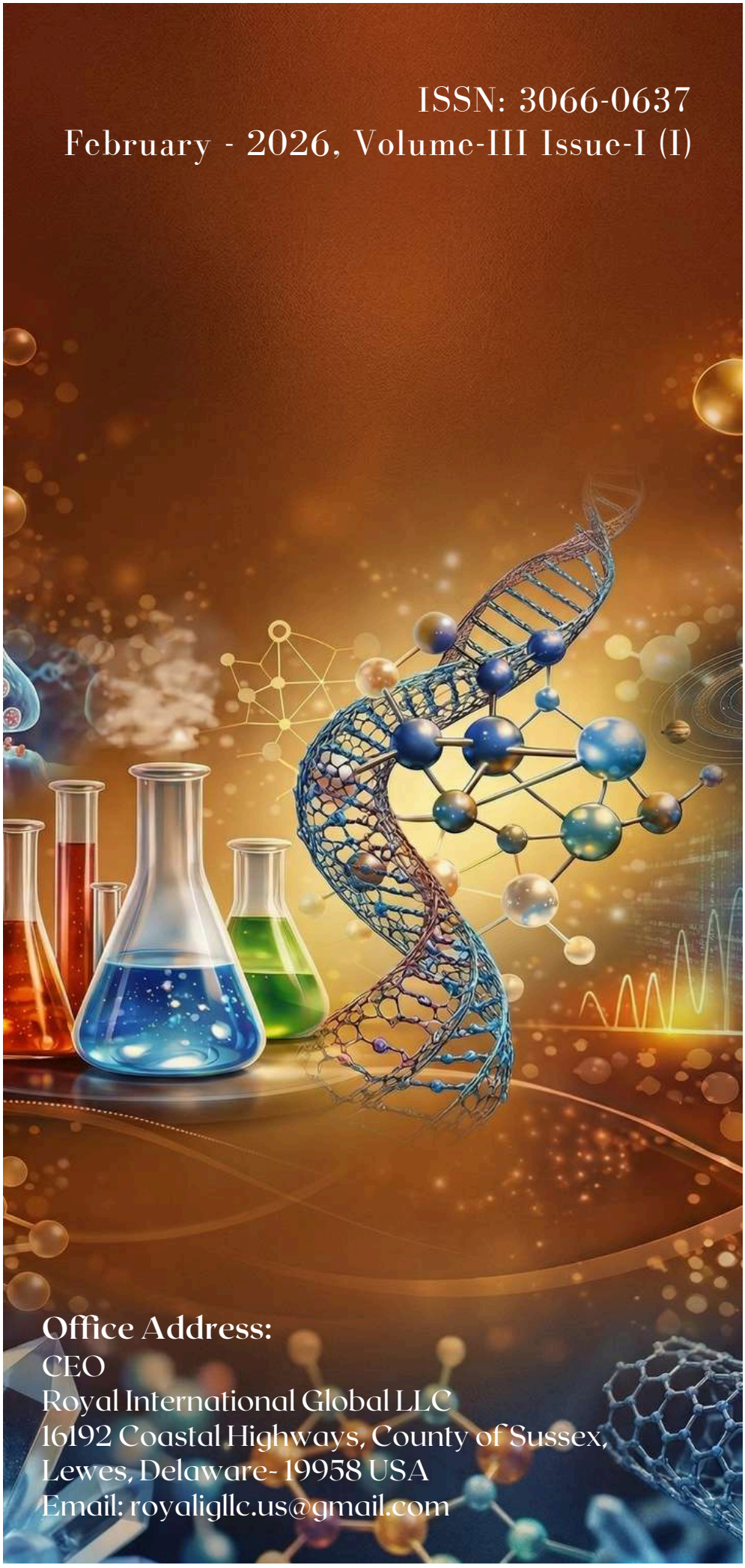
Double-blind peer-reviewed /refereed, open access online International journal

February - 2026
Volume-III Issue-I(I)

ISSN 3066-0637

9 773066 063005

ISSN: 3066-0637
February - 2026, Volume-III Issue-I (I)



Office Address:
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Royal International Global LLC
16192 Coastal Highways, County of Sussex,
Lewes, Delaware- 19958 USA
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Government Degree College for Women (A)
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Ramagiri, NALGONDA - 508 001 (T.G.)
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Proceedings

Of

TWO DAY INTERNATIONAL SEMINAR

ON

NEW VISTAS OF CHEMISTRY – AN INTERDISCIPLINARY APPROACH

(7th & 8th January 2026)

A Special Issue of Full-Length Articles

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International Journal of Research Studies on Environment, Earth, and Allied Sciences

ISSN: 3066-0637
Volume No-3, Issue-1(I), February 2026
Publication Language – English
Periodicity of Publication- Bi-Monthly
Email: esrd.us@gmail.com
Website: https://eesrd.us

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Name of Journal	**International Journal of Research Studies on Environment, Earth, and Allied Sciences**
Frequency	Bi-Monthly (February, April, June, August, October and December)
ISSN	3066-0637
Publisher	Royal International Global LLC 16192 Coastal Highway, County of Sussex, Lewes, Delaware 19958 USA
Chief Editor	Dr. Babalola, Ayodele Samuel
Copy right	Royal International Global LLC
Starting Year	October 2024
Subject	Multi-Disciplinary (Science Subject)
Review Process	Double Blind Review Process
Language	English
Publication Format	online
Access	OPEN ACCESS
License	Attribution-NonCommercial-ShareAlike 4.0 International
Phone No.	(+1) 3023033026
Email	esrd.us@gmail.com
Journal Website	https://eesrd.us
Registered office Address	CEO Royal International Global LLC 16192 Coastal Highway, County of Sussex, Lewes, Delaware 19958 United States of America (USA)
Admin. Office Address	CEO Royal International Global LLC 16192 Coastal Highway, County of Sussex, Lewes, Delaware 19958 United States of America (USA)

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International Journal of Research Studies on Environment, Earth, and Allied Sciences

ISSN: 3066-0637
Volume No-3, Issue-1(I), February 2026
Publication Language – English
Periodicity of Publication- Bi-Monthly
Email: esrd.us@gmail.com
Website: https://eesrd.us

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Principal.



Message

It gives me immense pleasure to present the Chemistry Proceedings – Special Issue comprising full-length research articles of the *Two-Day International Seminar on "New Vistas of Chemistry – An Interdisciplinary Approach"*, organized by the Department of Chemistry, Government Degree College for Women (Autonomous), Nalgonda, during **7–8 January 2026.**

The successful conduct of this international seminar reflects the institution's commitment to promoting academic excellence, research culture, and interdisciplinary learning. Chemistry, being a central science, plays a crucial role in addressing contemporary challenges related to sustainable development, environmental protection, healthcare, and technological advancements. The theme of the seminar aptly highlights the importance of integrating diverse scientific perspectives to foster innovation and problem-solving.

The publication of this proceedings volume is a significant academic milestone. It showcases the scholarly contributions of researchers, academicians, and students from various institutions, providing a valuable platform for dissemination of knowledge and exchange of ideas. I am confident that this special issue will serve as a useful reference for researchers and inspire further scientific inquiry.

I congratulate the Department of Chemistry for taking up this initiative and successfully organizing the seminar. I appreciate the dedicated efforts of the Convener, Organizing Committee, and Editorial Team in bringing out this proceedings volume with great commitment and precision.

I also extend my gratitude to all the speakers, participants, and contributors whose valuable inputs made this academic endeavor a grand success.

I wish this publication every success and hope it contributes meaningfully to the advancement of chemical sciences.

Principal,
Govt. Degree College for Women (Autonomous)
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Commissionerate of Collegiate Education



Prof. P. Balabhaskar
Joint Director

It gives me immense pleasure to extend my warm greetings and wholehearted support to the organizers, contributors, faculty members, and students on the successful organization of the Two-Day International Seminar on "New Vistas of Chemistry – An Interdisciplinary Approach", held on 7–8 January 2026, by the Department of Chemistry, Government Degree College for Women (Autonomous), Nalgonda, and the publication of the Chemistry Proceedings – Special Issue comprising full-length research articles.

In the present global scenario, Chemistry plays a pivotal role in addressing challenges related to sustainable development, environmental protection, healthcare innovations, and advanced materials. The interdisciplinary nature of modern chemical research continues to open new avenues for innovation and societal progress. The seminar has provided a valuable platform for academicians, researchers, scientists, and young scholars to exchange ideas, present their findings, and explore emerging trends in chemical sciences.

The publication of this proceedings volume is a commendable effort, reflecting the scholarly contributions and research excellence of the participants. It will serve as a significant academic resource for future research and learning.

I place on record my appreciation to the Principal for academic leadership and commend the Convener, Editorial Team, and Organizing Committee for their meticulous planning and dedicated efforts in successfully conducting the seminar and bringing out this special issue.

I am confident that this initiative will contribute to strengthening research culture and academic excellence in higher education.

Prof. P. Balabhaskar

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CHAIRMAN



MESSAGE

It gives me immense pleasure to extend my warm greetings and best wishes on the successful organization of the Two-Day International Seminar on ***"New Vistas of Chemistry – An Interdisciplinary Approach"*, held on 7–8 January 2026 by the Department of Chemistry, Government Degree College for Women (Autonomous), Nalgonda**.

Chemistry continues to remain a pivotal discipline driving advancements in sustainable technologies, pharmaceuticals, materials science, energy solutions, and environmental remediation. In today's rapidly evolving scientific landscape, the interdisciplinary integration of chemical sciences has become indispensable for addressing complex global and societal challenges.

This seminar has provided an excellent platform for intellectual exchange, fostering scholarly interaction and facilitating meaningful discussions on emerging trends and innovations in chemistry and allied domains. Such academic engagements significantly contribute to the advancement of knowledge and research.

I appreciate the exemplary academic leadership of the Principal and extend my congratulations to the Convener, Editorial Team, and Organizing Committee for their dedicated efforts in successfully organizing the seminar and bringing out this special issue.

I wish the Seminar great success and hope it will inspire continued research, innovation, and fruitful academic collaborations.

Warm regards,

(Prof. V. Balakista Reddy)

Index

Sr. No.	Paper Title	Page No.
1	Photocatalytic Degradation of Organic Dye Pollutants in Water Using La-Doped ZnO Nanocomposites Under Visible and Solar Light Irradiation **A. Vasantha, B. Vijayalaxmi, K. Venkatesham, A. Dayanand, A. Hari Padmasri**	**1-12**
2	Integrating Artificial Intelligence into Chemical Synthesis: Advances, Applications, and Challenges **Dr. Ashok Alishala, Dr. B. Ramesh**	**13-15**
3	DNA Interaction Profile of Newly Synthesized Ru (II) Complexes: Implications for Antimicrobial and Anti proliferative Activity **A. Dayanand, D. Venkateshwar Rao, R. Lavanya, K. Thirupathaih, A. Vasantha, N. Deepika**	**16-20**
4	Microplastic Pollution in Aquatic Ecosystems: A Comprehensive Review of Environmental Impacts and Potential Solutions **Mummadi Narsing Rao**	**21-29**
5	Validated Indirect Spectrophotometric Determination of Selected Drugs via Cerium (IV)–Methylene Blue Redox Reaction **Dr. Rajitha Balusani, Dr. Bandi Jyothi**	**30-33**
6	Green Chemistry as A Foundation for Sustainable Development: Innovations, Practices, And Global Implications **Dr. D. Valli Sowbhagyam, Dr. P. Vinod Kumar Goud**	**34-36**
7	Applications of Superconductivity in Medicine, Power Systems, and Transportation: A Comprehensive Review **K. Naresh, V. Shekar, D. Bala Narsimha, M. Nagu**	**37-41**
8	Effect of Co-Mo nitride catalyst over carbonaceous support in the Oxidative dehydrogenation of Ethylbenzene **Dr J. Madhavi**	**42-45**
9	Forever Chemicals (PFAS): Environmental Persistence and Chemical Remediation Strategies **D. Venkateshwar Rao, A Dayanand**	**46-48**
10	Diatom Diversity and Physico-Chemical Characteristics of a Freshwater Lake in Sangareddy District, Telangana, India **Dr. K. Anuradha**	**49-52**
11	New Vistas of Chemistry—An Interdisciplinary Approach: Phyto-Mediated Synthesis of Silver Nano-Particles (Agnps) **Dr. L. Kamala**	**53-56**
12	Applications of Nanotechnology for Environmental Remediation **Dr. K. Lakshmi Prameela, K. Anusha**	**57-60**
13	Biophysical Characterization of Drug–Protein Interactions through UV, Fluorescence, and Circular Dichroism Spectroscopy **M. Prabhavathi, Dr. Suprabha Panda**	**61-64**
14	Nano material Synthesis and Characterization for Catalytic and Renewable Energy Applications **Dr. Rekha Venkateswarlu**	**65-68**
15	Assessment of Composition of Selected Heavy Metals in Road Dust from Sangareddy Region **Dr. Abhijit Kantankar, Dr. M. Sunitha**	**69-74**
16	Microplastics and Nanoplastics in the Environment: Chemical and Biochemical Strategies for Effective Degradation **V. Sahiti, P. Pushpalatha**	**75-78**
17	Green Solvents and Their Impact on Sustainable Chemical Process Design: A Review **Dr. V. Saritha Rani**	**79-82**
18	Sustainable Waste Management in India: Strategies and Solutions **Devarinti Srihari Reddy**	**83-87**

19	1-Butyl-1-methylpyrrolidinium-1,2,4-triazolide ([BMP][Tz]): A Novel Ionic Liquid Solvent for Catalyst-Free N-tert-Boc Protection of Amines under Mild Conditions **Vanam Shekhar, Dhoddi Bala Narsimha, Pingili Upendra, Kurapati Ravi, Kommu. Naresh**	**88-91**
20	Narrative Alchemy: Transmuting Text through Chemical Lenses **Y. Chaitanya Sudha**	**92-94**
21	Role of Si/Al ratio in the Valorization of Glycerol to a Fuel Additive, Solketal over HZSM-5 Catalysts **Yadaiah Salwadi, Venkatesham Kothabai, Vijayalaxmi Burri, Balakrishna Matkala, Sasikumar Boggala, Hari Padmasri Aytam**	**95-102**
22	Computational Chemistry Approaches to Capturing Polluted Air and Converting It into Environment-Friendly Gases **Vijaya Belamkonda**	**103-107**
23	New Vistas of Chemistry: An Interdisciplinary Approach **Dr. Ambala Sudarshan**	**108-110**
24	The Role of Mathematics in Chemistry **Venkateshwarlu**	**111-113**
25	Synthesis, Spectroscopic Characterization and DPPH Radical Scavenging a Vanillin-Derived Schiff Base **Dr. Nirupa Gadapa**	**114-119**
26	Biofuel Generations and Its Impact on the Environment **Archana Garipelly**	**120-122**
27	Eat Right for a Better Life: A Survey on Dietary Practices and Lifestyle Patterns **Dr. P. Latha**	**123-126**
28	Viksit Bharat (Developed India)- An Integrated Perspective of Botany and Chemistry **Dr. B. Sofia Rani**	**127-131**

International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030101

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465001

DOI Link:
https://doi.org/10.5281/zenodo.19465001

Volume: 3

Issue: 1(I)

Pp. 1-12

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 10 Jan. 2026

Revised: 20 Jan. 2026

Accepted: 03 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
A. Vasantha, B. Vijayalaxmi, K. Venkatesham, A. Dayanand, & Padmasri, A. H. (2026). Photocatalytic Degradation of Organic Dye Pollutants in Water Using La-Doped ZnO Nanocomposites Under Visible and Solar Light Irradiation. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 1–12. https://doi.org/10.5281/zenodo.19465001

Photocatalytic Degradation of Organic Dye Pollutants in Water Using La-Doped ZnO Nanocomposites Under Visible and Solar Light Irradiation

A. Vasantha[1], B. Vijayalaxmi[2], K. Venkatesham[3], A. Dayanand[4], A. Hari Padmasri[5]
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Abstract

ZnO stands out as one of the most widely employed photocatalysts among n-type semiconductors, owing to its favorable physicochemical attributes including its band gap, binding energy, room-temperature optical gain, non-toxicity, biocompatibility, and cost-effectiveness. The f-orbital interactions of rare earth elements with functional groups present in dyes enable complex formation and effectively reduce the photocatalyst band gap upon doping. In this investigation, nano ZnO was functionalized by incorporating Lanthanum (La) at varying concentrations from 1 to 5 wt.% via the sol-gel technique. The physicochemical properties—including crystal structure, morphology, surface area, absorption maximum, band gap, emission characteristics, and surface composition—of the synthesized nano ZnO and La-doped nano ZnO were thoroughly analyzed using a range of characterization techniques. XRD data confirmed retention of the ZnO Wurtzite hexagonal phase across all La-doped samples; the average crystallite size progressively diminished from 19.5 to 9.8 nm as La content rose from 1 to 5 wt.%, while the band gap (determined by UV-DRS) decreased correspondingly. Photoluminescence (PL) intensity also declined with increasing La content. The photodegradation performance of the synthesized photocatalysts was evaluated against organic dye solutions. All tested catalysts retained consistent activity across five successive reaction cycles. Radical trapping experiments using appropriate scavengers confirmed that photogenerated electron-hole pairs, superoxide radicals, and hydroxyl radicals participate in the degradation pathway.

Keywords: *La-doped ZnO nanocomposites; photodegradation; organic dyes; visible light irradiation*

Introduction

Incorporating metallic ions into the ZnO crystal lattice [1–4] imparts enhanced optical, magnetic, and electrical properties, making ZnO-based materials suitable for diverse applications including magnetic semiconductors, solar cells, field-effect transistors, gas sensors, light-emitting devices, photocatalysts, and biological systems such as bio-imaging and drug delivery platforms [5, 6]. Of particular interest is the substitution of rare earth elements (e.g., La, Tb, Er, Eu, Dy, and Sm) into the ZnO lattice, which confers significant advantages, including improved photocatalytic activity [7].

The present study employs multiple characterization approaches: XRD for crystal structure identification, BET surface area analysis, UV-DRS for optical property determination and band gap energy calculation, SEM-EDAX for morphological and elemental analysis, and XPS for surface chemical composition. These are complemented by photocatalytic degradation studies using brilliant yellow and acid blue dyes as model pollutants.

Experimental

Synthesis of La-Doped ZnO Photocatalysts: 21.63 g of $Zn(NO_3)_2 \cdot 6H_2O$ was dissolved in 100 mL of distilled water, and 0.5 g of La $(NO_3)_3 \cdot 5H_2O$ in 50 mL of distilled water. Both solutions were blended dropwise with continuous stirring and subsequently combined with a citric acid solution. The pH was adjusted to 7 by the gradual addition of ammonia solution. The mixture was then heated to 80 °C to form a gel, which was filtered, washed, and dried at 100 °C overnight, followed by calcination at 500 °C for 4–5 hours [8]. The resulting catalysts were designated 1LZ through 5LZ corresponding to 1–5 wt.% La loading.

Characterization: Powder X-ray diffraction (XRD) patterns were collected on a Rigaku Miniplex diffractometer. Nitrogen adsorption measurements provided surface area data, while morphology and elemental distribution were examined by field emission scanning electron microscopy (FE-SEM) coupled with energy dispersive X-ray (EDX) analysis.

UV-vis diffuse reflectance spectra (UV-vis DRS) were acquired using a JASCO V650 spectrophotometer. Photoluminescence (PL) emission spectra were recorded at room temperature using a JASCO FP-8500 spectrofluorometer with an excitation wavelength of 220 nm.

Photocatalytic Degradation Studies: Degradation experiments were performed in a reactor under visible light irradiation. Efficiency was tracked by measuring absorbance changes of brilliant yellow and acid blue dye solutions at 30-minute intervals. Details of the experimental configuration are reported elsewhere [9]. Degradation efficiency D (%) was calculated as:

$$D\ (\%) = [(C_0 - C) / C_0] \times 100 = [(A_0 - A) / A_0] \times 100$$

where C_0 and A_0 are the initial dye concentration and absorbance, and C and A are the corresponding values at each 30-minute measurement interval.

Results and Discussion

X-Ray Diffraction (XRD)

XRD analysis (Fig. 1) confirmed that all samples retained the characteristic hexagonal wurtzite crystal structure of ZnO. No secondary phases or impurities were detected, verifying the clean incorporation of La into the ZnO host lattice. A systematic broadening and attenuation of the primary diffraction peak were observed as La loading increased, consistent with a reduction in crystallite size (Table 1). This trend indicates that higher La concentrations suppress crystallite growth within the La-ZnO framework [10].

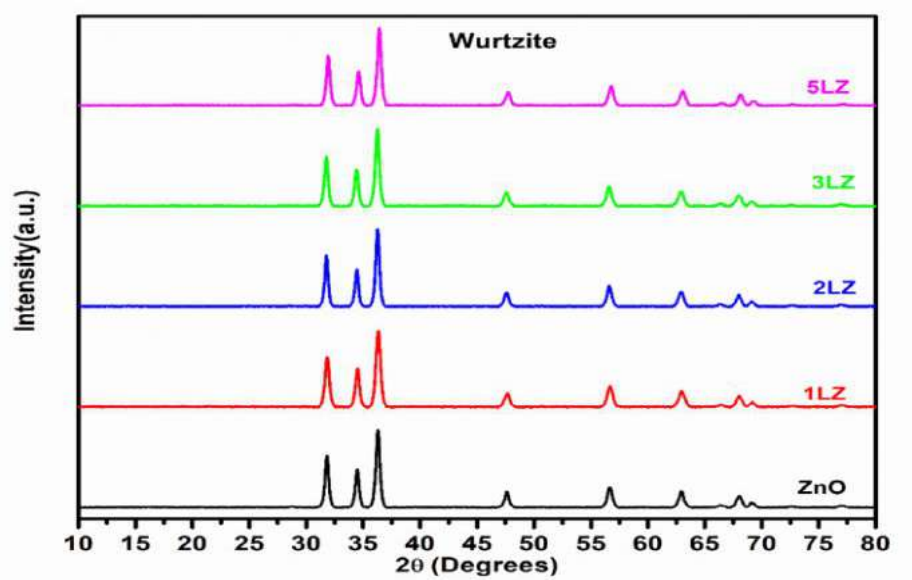


Figure 1: XRD Patterns of ZnO and 1, 2, 3, and 5 wt.% LZ Nanocomposites

Table 1: Physicochemical Properties of the Synthesized Nano Photocatalysts

Catalyst	2θ (degrees)	Crystallite Size (nm)	BET-SA ($m^2g^{-1}_{tat}$)	UV-DRS Absorption Edge (nm)	Band Gap (eV)
ZnO	36.324	19.5	14.231	450	3.23
1LZ	36.293	18.9	13.581	455	3.01
2LZ	36.283	12.1	16.789	466	2.88
3LZ	36.270	10.3	19.289	473	2.81
5LZ	36.147	9.8	23.782	477	2.75

BET Surface Area Analysis

The BET surface areas measured for ZnO and 1–5 wt.% La-ZnO were 14.231, 13.581, 16.789, 19.289, and 23.782 m^2g^{-1}, respectively (Table 1). This progressive rise in specific surface area upon La doping reflects the inhibitory effect of La on-crystallite growth, stabilization of the wurtzite phase, and increased mesoporosity. Nitrogen adsorption isotherms (not shown) exhibited Type IV behavior, with La-ZnO samples displaying H_2-type hysteresis, characteristic of capillary condensation in mesoporous architectures [11].

SEM-EDAX Analysis

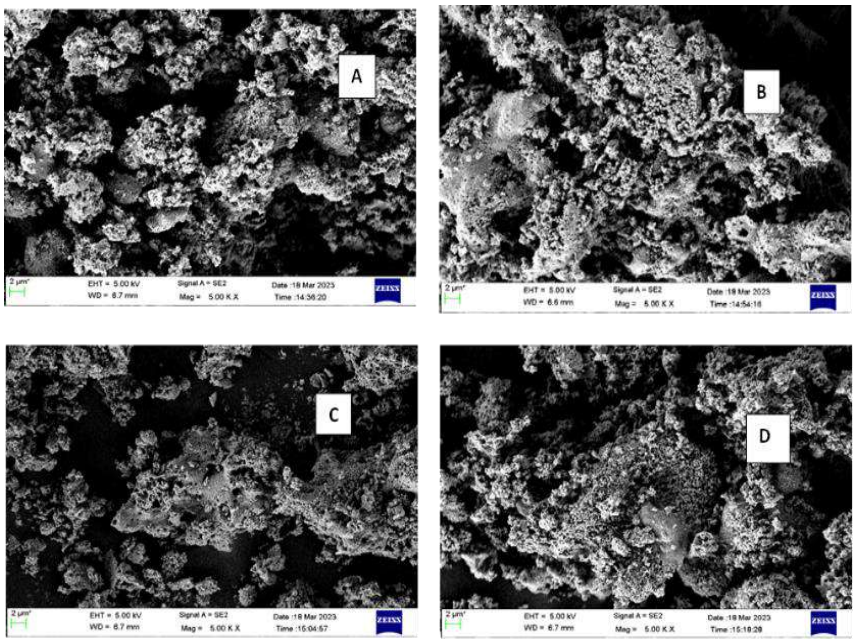


Figure 2: SEM Micrographs of A) 1 wt.% LZ B) 2 wt.% LZ C) 3 wt.% LZ D) 5 wt.% LZ

SEM images (Fig. 2) reveal that La doping progressively reduces semiconductor crystallite dimensions, with particles adopting a predominantly spherical morphology. The presence of La at intercrystallite boundaries inhibited direct contact and impeded particle coarsening, thereby promoting smaller grain sizes [12]. EDAX spectra (Fig. 3, Table 2) corroborate the successful incorporation of La at the intended concentrations on the ZnO surface.

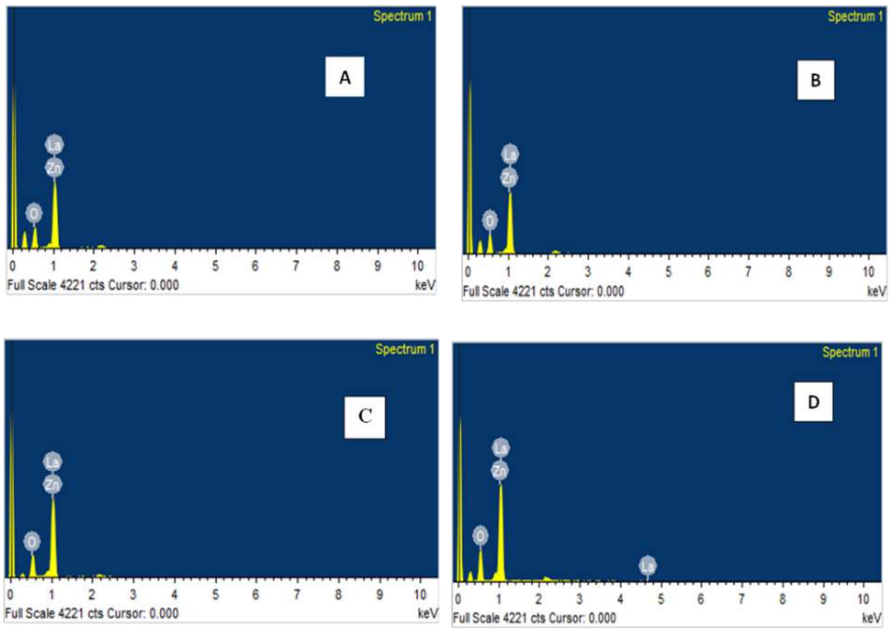


Figure 3: EDAX Spectra and Elemental Composition of A) 1 wt.% LZ B) 2 wt.% LZ C) 3 wt.% LZ D) 5 wt.% LZ

Table 2: EDAX Elemental Composition of La-ZnO Nanocomposites

A) 1 Wt.% La-ZnO			B) 2 Wt.% La-ZnO		
Element	**Weight%**	**Atomic%**	**Element**	**Weight%**	**Atomic%**
O K	22.54	53.95	O K	21.24	52.81
Zn L	75.31	46.46	Zn L	76.46	46.53
La L	2.15	0.59	La L	2.30	0.66

Total	100.00		Total	100.00	
C) 3 Wt.% La-ZnO			**D) 5 Wt.% La-ZnO**		
Element	**Weight%**	**Atomic%**	**Element**	**Weight%**	**Atomic%**
O K	19.52	50.27	O K	20.48	51.79
Zn L	77.52	48.86	Zn L	76.50	47.34
La L	2.96	0.87	La L	3.01	0.88
Total	100.00		Total	100.00	

TEM Analysis

TEM imaging (Fig. 4) for the 5% La-ZnO sample illustrates particles with comparable shapes but varying dimensions. The synthesized nanoparticles showed a size distribution in the range of 15–25 nm, with a mean particle diameter of approximately 19 nm. Incorporation of La^{3+} narrowed the particle size distribution relative to undoped ZnO [10]. The selected area electron diffraction (SAED) pattern of 5% LZ exhibits concentric diffraction rings consistent with the hexagonal wurtzite crystal structure.

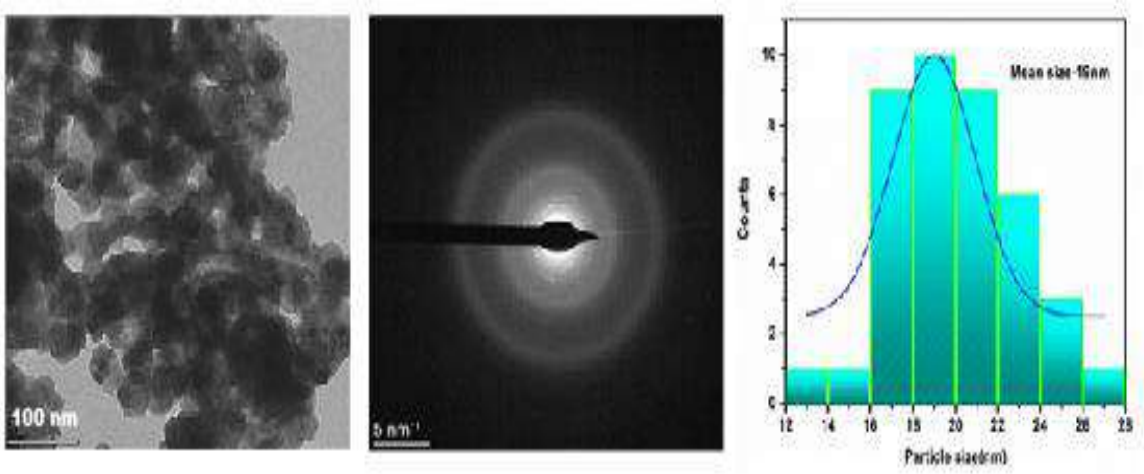


Figure 4: TEM Image, SAED Pattern, and Particle Size Distribution Histogram of 5% LZ

UV-DRS and Photoluminescence Analyses

All ZnO and 1–5 wt.% La-ZnO nanocomposites displayed absorbance in the 400–480 nm region (Fig. 5A). Band gap energies derived from Kubelka-Munk (KM) plots (Fig. 5B) ranged from 3.23 to 2.73 eV for ZnO and 1–5 wt.% LZ, respectively (Table 1). These spectral results confirm that La^{3+} doping induces a systematic red shift in the absorption edge, extending from 1 wt.% to 5 wt.% La-ZnO, accompanied by a reduction in band gap energy [7].

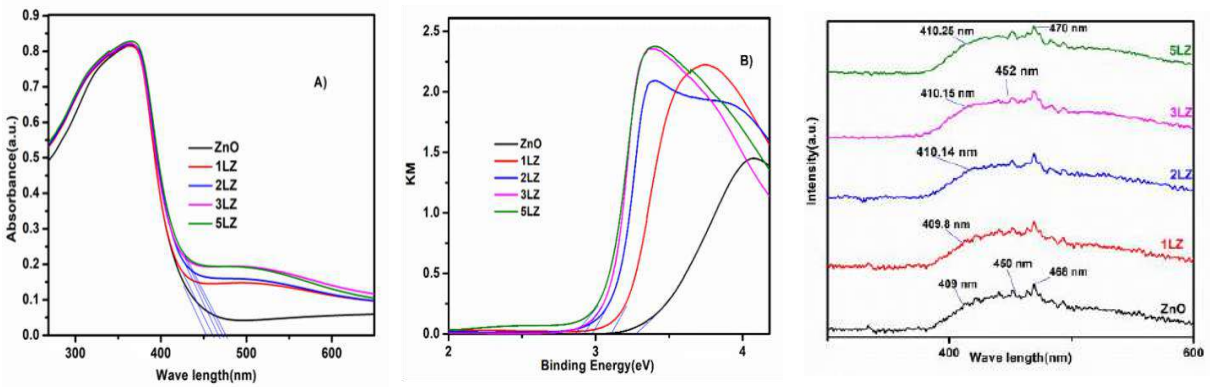


Figure 5: (A) UV-Vis DRS Spectra; (B) Kubelka-Munk Plot; (C) PL Spectra of ZnO and 1–5 LZ

Nanocomposites

PL emission spectra revealed peaks at 409, 450, and 468 nm for ZnO, and at 410.25, 452, and 470 nm for 1–5 wt.% La-ZnO. Emissions in the visible region arise from the recombination of holes with electrons in singly

ionized oxygen vacancy states [14, 15]. The relationship between PL characteristics and crystallinity indicates that lower defect density yields better crystallinity [16]. The observed decline in PL intensity with increasing La content is inversely correlated with photocatalytic activity. Narrowing of the band gap is attributed to a transition shift from O 2p to La 3d (instead of Zn 2p as in pristine ZnO) [15]. Being less electronegative than Zn^{2+} on the Pauling scale, La^{3+} forms isoelectronic bonds that trap electron-hole pairs and generate La^{2+}, which in turn captures electrons and creates acceptor-bound excitons through Coulombic interactions. The corresponding trapping of adsorbed molecular oxygen can be expressed as:

$$La^{3+} + e^- \rightarrow La^{2+}$$
$$La^{2+} + O_2 \rightarrow La^{3+} + {\bullet}O_2^-$$

X-Ray Photoelectron Spectroscopy (XPS)

Wide-scan XPS spectra (Fig. 6A) of ZnO and 1–5 wt.% La-ZnO display peaks attributable to Zn and O, reflecting their abundance on the catalyst surface. The absence of La-related peaks in wide scans is consistent with the low La loading relative to Zn and O. High-resolution Zn 2p spectra (Fig. 6B) show Zn $2p_{3/2}$ and Zn $2p_{1/2}$ peaks at 1018 and 1042 eV for ZnO, shifting to 1022 and 1045 eV for 5 wt.% La-ZnO. These binding energies correspond to Zn^{2+} in the Zn-O bond, with the observed shift primarily attributed to Zn-O-La bonding and progressively extending to higher binding energies with increasing La content [13]. La 3d XPS peaks (Fig. 6C) appear at 835.7 and 852 eV for $3d_{3/2}$ and $3d_{5/2}$ respectively, consistent with La^{3+} species and in agreement with reference binding energy values. The O 1s spectrum (Fig. 6D) for ZnO exhibits a peak at 527.5 eV (Zn-O-Zn), while the broader O 1s feature in La-ZnO is deconvoluted into two components at 530.5 and 531.8 eV, ascribed to chemisorbed hydroxyl groups and surface-adsorbed oxygen species, respectively [14].

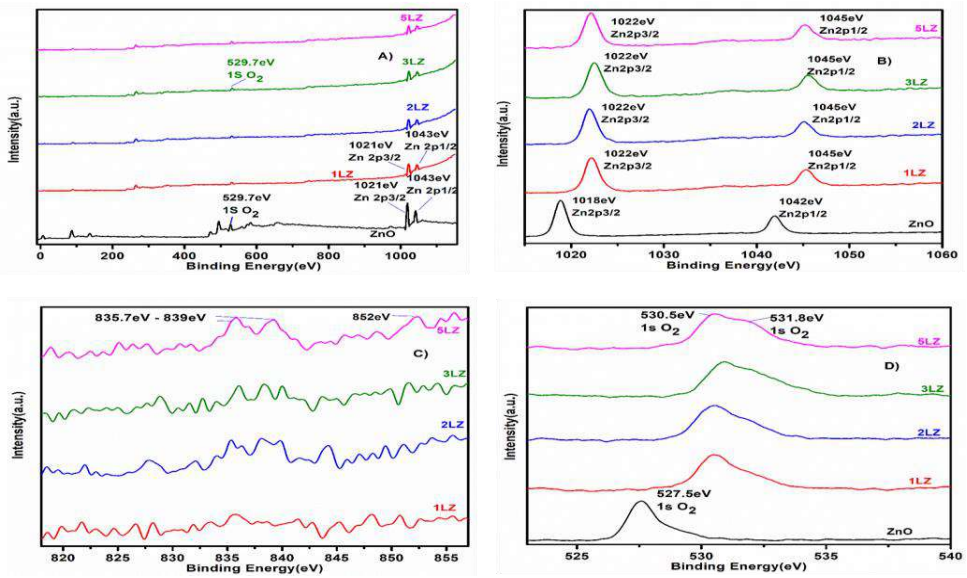


Figure 6: XPS Spectra of ZnO and 1–5 wt.% LZ Nanocomposites: (A) Wide Scan; (B) Zn 2p; (C) La 3d; (D) O 1s

Photocatalytic Degradation Performance

Photocatalytic efficiency toward brilliant yellow and acid blue dye degradation improved systematically from bare ZnO to 5 wt.% La-ZnO. The initial stage involves adsorption and accumulation of dye molecules onto the nanoparticle surface under irradiation. Continuous migration of reactants and successive photocatalytic oxidation at the nanoparticle surface contribute to the observed gains in degradation efficiency.

Visible Light Photocatalysis

Among all tested catalysts, the 5 wt.% La-ZnO nanocomposite achieved the highest degradation efficiencies of 84% and 89% for brilliant yellow and acid blue dyes, respectively (Figs. 7 and 8, Table 3). Notably, 75 mg of La-doped ZnO catalyst applied to 50 ppm acid blue yielded an exceptional 89% degradation efficiency (Fig. 8E), confirming a positive correlation between La content and photocatalytic performance.

Table 3: Photocatalytic Degradation Efficiency (%) of Dyes Over La-ZnO Nanocomposites Under Visible and Solar Light

Catalyst	Visible Light: Brilliant Yellow Dye (%)	Visible Light: Acid Blue Dye (%)	Sunlight: Brilliant Yellow Dye (%)	Sunlight: Acid Blue Dye (%)
Bare ZnO	28	24	28.9	34.1
1LZ	36	39	44.3	45
2LZ	54	59	66	50.4
3LZ	68	72	69.7	63
5LZ	84	89	93.6	72.1

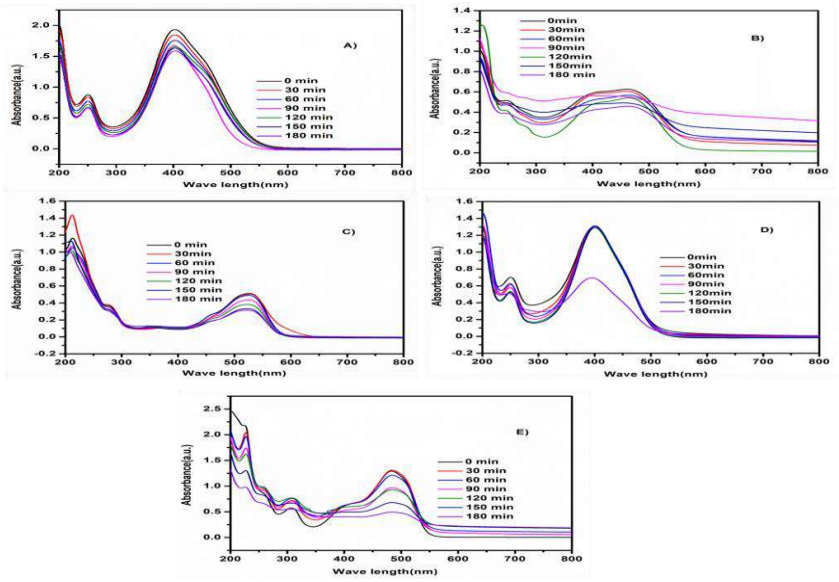


Figure 7: Photodegradation of 50 ppm Brilliant Yellow Dye Using 75 mg Catalyst in Visible Light Over A) ZnO B) 1 wt.% LZ C) 2 wt.% LZ D) 3 wt.% LZ E) 5 wt.% LZ

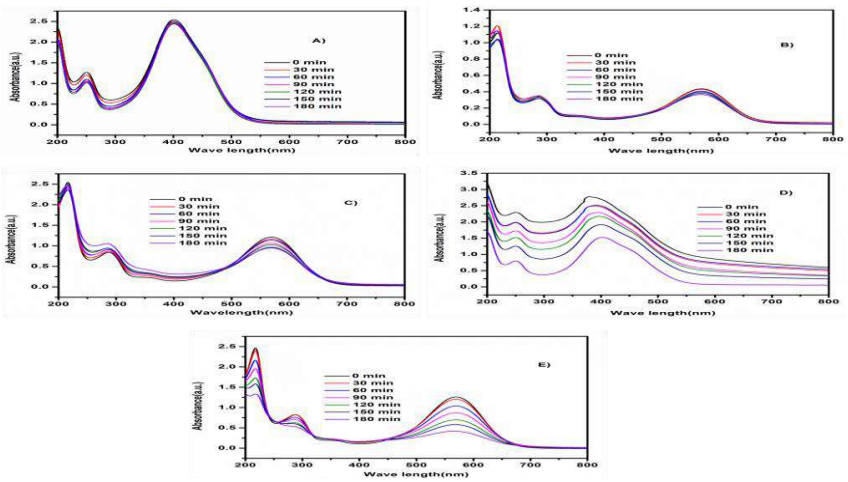


Figure 8: Photodegradation of 50 ppm Acid Blue Dye Using 75 mg Catalyst in Visible Light Over A) ZnO B) 1 wt.% LZ C) 2 wt.% LZ D) 3 wt.% LZ E) 5 wt.% LZ

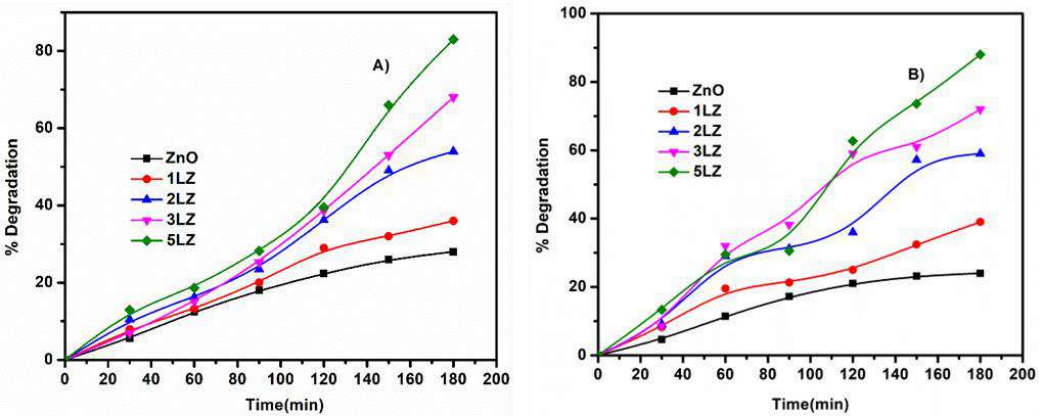


Figure 9: % Photodegradation of A) Brilliant Yellow B) Acid Blue in Visible Light Over ZnO and 1–5 wt.% LZ

Dye degradation kinetics conformed to a pseudo-first-order reaction model (Figs. 10A and B), as documented in comparable studies [15, 16]. Rate constants and regression coefficients (R^2) for both dyes over ZnO and 1–5 wt.% La-ZnO are provided in Table 4. The progressive enhancement in rate constants with increasing La loading underscores the intrinsic photocatalytic improvement brought about by La doping [17].

Table 4: Rate Constants and R^2 Values for Photodegradation of Brilliant Yellow and Acid Blue Dyes in Visible Light

Catalyst	Brilliant Yellow: k (min^{-1})	R^2	Acid Blue: k (min^{-1})	R^2
ZnO	1.20×10^{-2}	0.9210	1.30×10^{-2}	0.9024
1 wt.% La-ZnO	1.41×10^{-2}	0.9361	1.48×10^{-2}	0.9428
2 wt.% La-ZnO	1.52×10^{-2}	0.9944	1.62×10^{-3}	0.9802
3 wt.% La-ZnO	1.64×10^{-2}	0.9899	1.80×10^{-2}	0.9929
5 wt.% La-ZnO	2.04×10^{-2}	0.9301	2.10×10^{-2}	0.9979

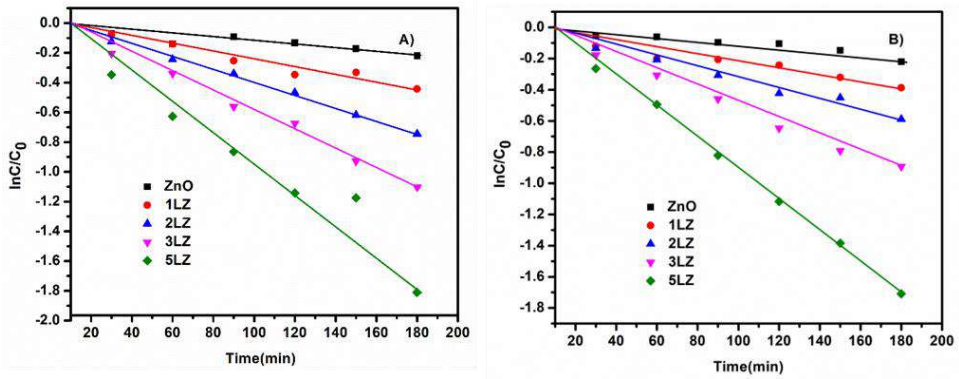


Figure 10: Degradation Kinetics of A) Brilliant Yellow B) Acid Blue in Visible Light Over ZnO and 1, 2, 3, and 5% LZ

Solar Light Photocatalysis

Photodegradation under sunlight (Figs. 11(i) and (ii)) followed similar trends, with 5 wt.% La-ZnO outperforming all other catalysts. Sunlight-driven degradation of brilliant yellow reached approximately 93%, compared to about 72% for acid blue, reinforcing the superior photocatalytic activity of La-doped ZnO over the undoped counterpart.

Rate constants and R^2 values under sunlight for both dyes across ZnO and 1–5 wt.% La-ZnO are summarized in Table 5. These values indicate consistently higher degradation rates under sunlight compared to visible light irradiation.

Table 5: Rate Constants and R^2 Values for Photodegradation of Brilliant Yellow and Acid Blue Dyes in Sunlight

Catalyst	Brilliant Yellow: k (min^{-1})	R^2	Acid Blue: k (min^{-1})	R^2
ZnO	1.31×10^{-2}	0.9834	1.40×10^{-2}	0.9981
1 wt.% La-ZnO	1.43×10^{-2}	0.9551	1.52×10^{-2}	0.9986
2 wt.% La-ZnO	1.58×10^{-2}	0.9901	1.60×10^{-2}	0.9819
3 wt.% La-ZnO	1.70×10^{-2}	0.9944	1.80×10^{-2}	0.9967
5 wt.% La-ZnO	2.00×10^{-2}	0.9861	2.02×10^{-2}	0.9980

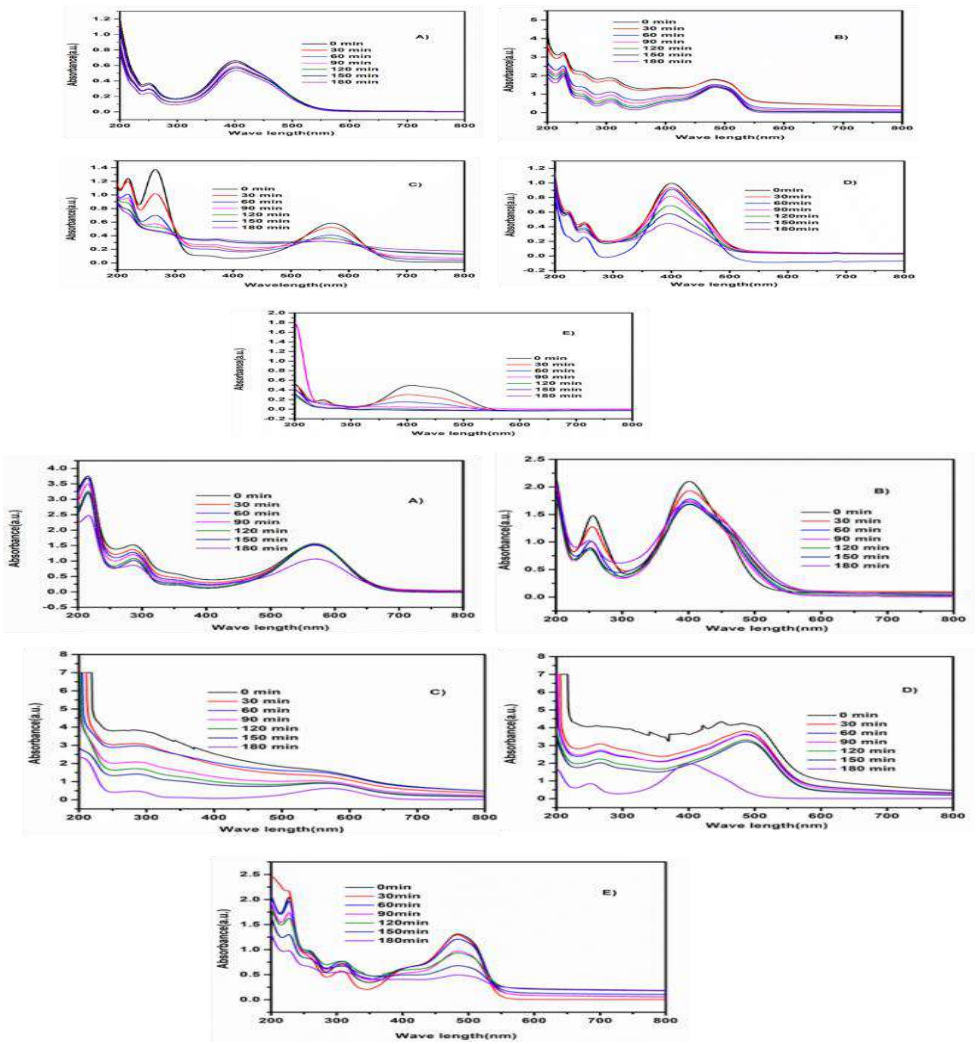


Figure 11: Photodegradation of 20 ppm (i) Brilliant Yellow Dye and (ii) Acid Blue Dye Under Sunlight Using 50 mg of A) ZnO B) 1LZ C) 2LZ D) 3LZ E) 5LZ

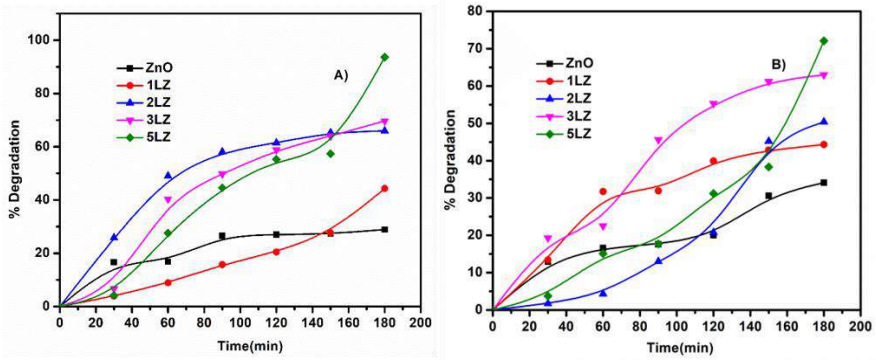


Figure 12: % Photodegradation of A) Brilliant Yellow B) Acid Blue Under Sunlight Over ZnO and 1, 2, 3, and 5% La-ZnO

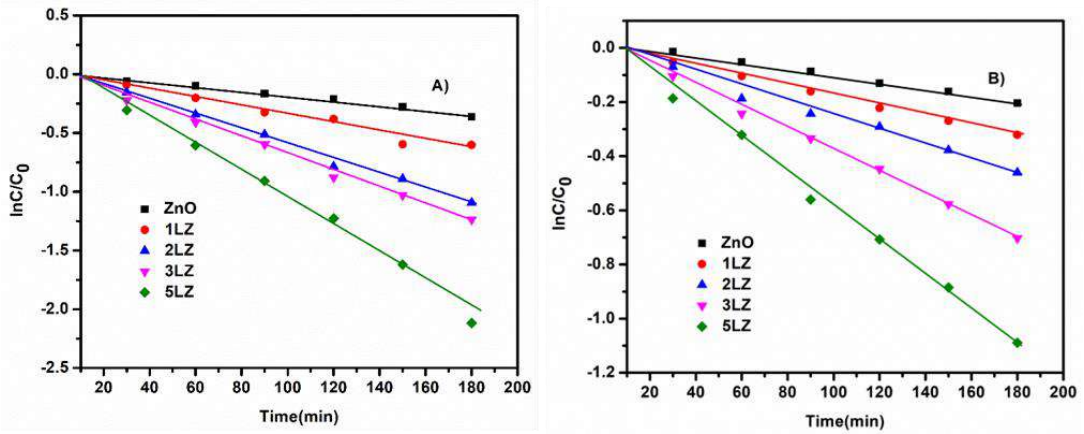


Figure 13: Degradation Kinetics of A) Brilliant Yellow B) Acid Blue Under Sunlight Over ZnO and 1, 2, 3, and 5% LZ

Reusability and Stability of Catalysts

Catalyst reusability was assessed over five consecutive reaction cycles in visible light (Fig. 14). Brilliant yellow degradation declined marginally from 84% to 81%, while acid blue degradation decreased from 89% to 84%, demonstrating robust catalytic stability across multiple uses. Comparable stability was also confirmed under sunlight (Fig. 15), with BY degradation declining slightly from 93% to 88% and AB degradation from 72% to 69%. Post-reaction XRD analysis of the used catalyst (Fig. 16A) confirmed that the crystal structure remained unchanged after five cycles, corroborating the material's structural robustness.

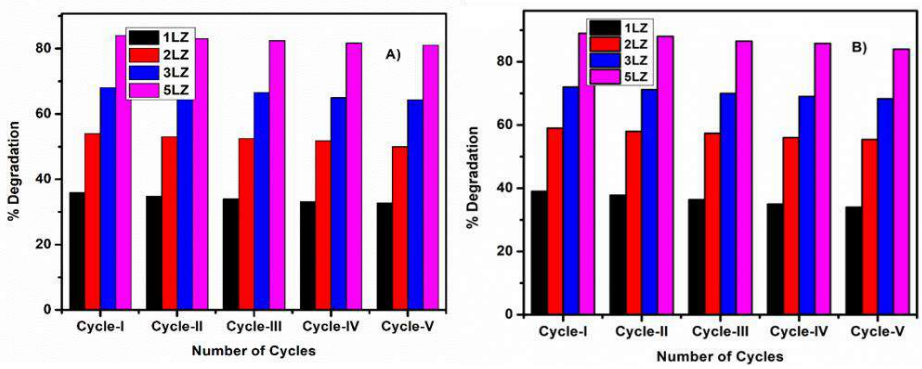


Figure 14: Reusability of La-ZnO Nanocomposites in Photodegradation of A) Brilliant Yellow B) Acid Blue Under Visible Light

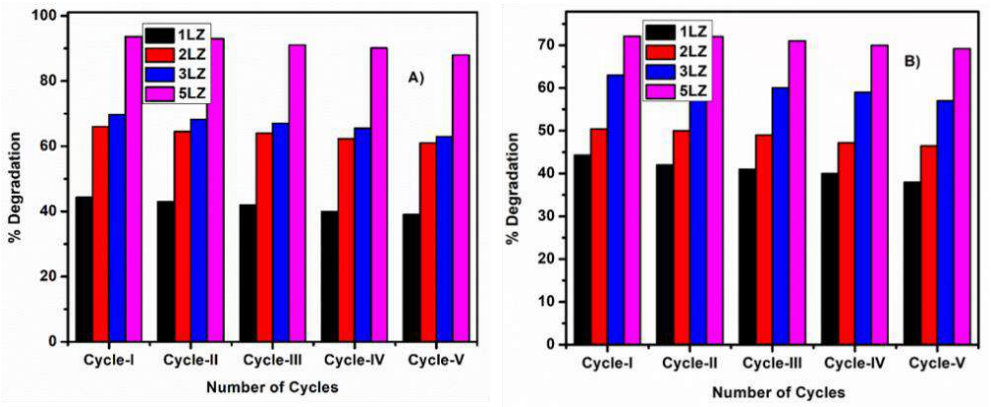


Figure 15: Reusability of LZ Nanocomposites in Photodegradation of A) Brilliant Yellow B) Acid Blue Under Sunlight

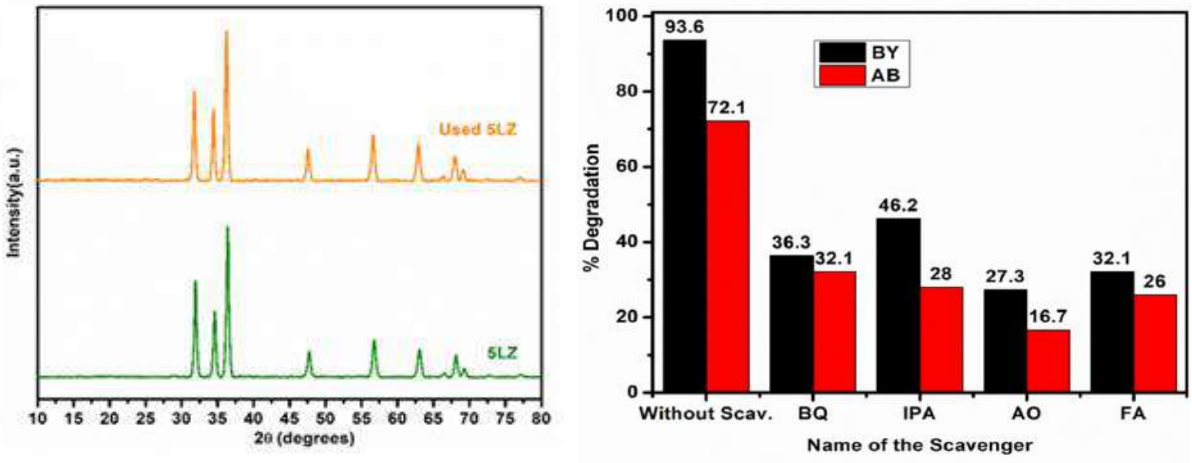
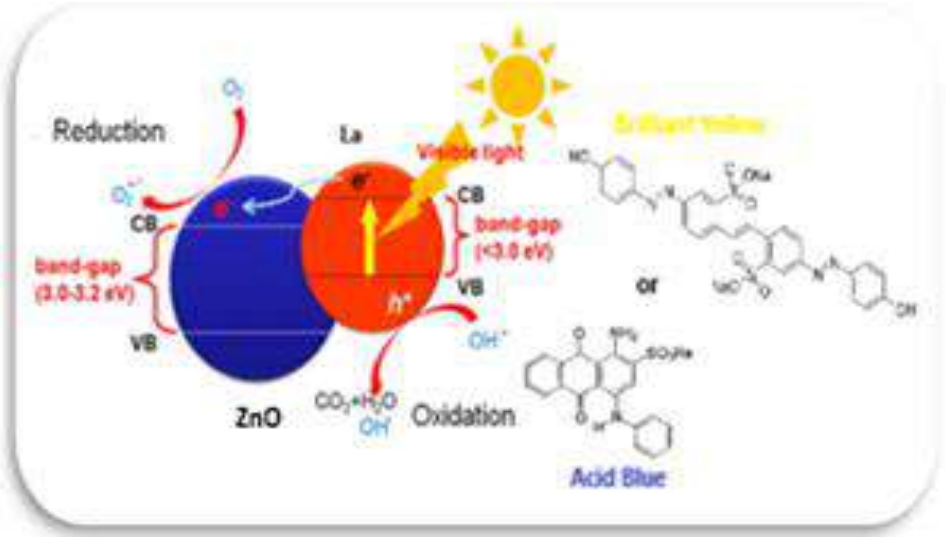


Figure 16: A) XRD Patterns of Fresh and Used 5LZ Catalyst; B) Effect of Scavengers (Benzoquinone, Isopropanol, Ammonium Oxalate, Formic Acid) on Photodegradation of Dyes Under Sunlight

Scavenger Studies

The roles of reactive species in the photocatalytic process were established through scavenger experiments [18, 19]. As shown in Fig. 16B, hole (h^+) scavengers—ammonium oxalate and formic acid—produced greater suppression of degradation activity than hydroxyl radical scavenger (isopropanol) and superoxide scavenger (benzoquinone) for both brilliant yellow and acid blue dyes over 5 wt.% La-ZnO under sunlight. This result indicates that holes are the primary reactive species governing the photocatalytic degradation mechanism.

Proposed Photocatalytic Mechanism



La doping narrows the band gap of ZnO, facilitating photon absorption in the visible region. Upon light exposure, electrons are excited from the valence band (VB) to the conduction band (CB), generating electron-hole pairs. Holes in the VB participate in oxidative reactions forming hydroxyl radicals (•OH), while CB electrons engage in reductive processes yielding superoxide radicals ($•O_2^-$). Both radical species possess sufficient redox potentials to decompose organic pollutants. Electron-donating azo groups (-N=N-) and unsaturated -C=C- bonds in the dye molecules are particularly susceptible targets for hydroxyl radical attack, ultimately leading to their mineralization [20]. The incorporation of a La-derived dopant

energy level within the band gap is responsible for the red-shifted absorption observed in UV-DRS spectra. Additionally, La modification suppresses electron-hole recombination, contributing to the enhanced photocatalytic degradation rates.

Conclusions

La-ZnO nanocomposites prepared by the sol-gel route demonstrated high photocatalytic activity in degrading brilliant yellow and acid blue dyes. Degradation efficiency increased with La loading, reaching a maximum at 5 wt.%. The nanocomposites maintained elevated performance even at higher dye concentrations, underscoring their applicability in real wastewater treatment scenarios. XRD and SEM characterization confirmed nanocrystalline particle dimensions and spherical morphology, while UV-DRS analysis evidenced a significant reduction in band gap upon La incorporation—all contributing factors to the enhanced photocatalytic performance. The 5LZ catalyst demonstrated superior photodegradation activity for both dyes under both visible and solar light, with reaction rates following the order:

k(BY) sunlight > k(BY) visible light > k(AB) sunlight > k(AB) visible light

The catalyst maintained consistent activity over five consecutive runs, establishing its reliability as a visible/solar-light-driven photocatalyst for organic dye degradation. These findings highlight the promise of La-doped ZnO nanocomposites as efficient, durable photocatalytic materials for environmental applications including wastewater remediation and organic pollutant removal.

Acknowledgment

I would like to express my sincere gratitude to all those who have contributed to the successful completion of this research work titled "Photocatalytic Degradation of Organic Dye Pollutants in Water Using La-Doped ZnO Nanocomposites Under Visible and Solar Light Irradiation."

First and foremost, I am deeply indebted to my project guide for their invaluable guidance, constant encouragement, and insightful suggestions throughout the course of this study. Their expertise and support have been instrumental in the successful execution of this research.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030102

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465083

DOI Link:
https://doi.org/10.5281/zenodo.19465083

Volume: 3

Issue: 1(I)

Pp. 13-15

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 10 Jan. 2026

Revised: 20 Jan. 2026

Accepted: 03 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Alishala, A., & B. Ramesh. (2026). Integrating Artificial Intelligence into Chemical Synthesis: Advances, Applications, and Challenges. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 13–15. https://doi.org/10.5281/zenodo.19465083

Integrating Artificial Intelligence into Chemical Synthesis: Advances, Applications, and Challenges

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Abstract

Artificial Intelligence (AI) is redefining the landscape of chemical synthesis by introducing data-driven models for retrosynthetic planning, reaction prediction, optimization, and automated experimentation. With recent advancements in machine learning (ML), graph neural networks (GNNs), large language models (LLMs), and self-driving laboratories (SDLs), chemical discovery is becoming faster, greener, and more reproducible. This paper reviews current progress (2023–2026) in AI-assisted synthesis, highlighting recent breakthroughs, case studies, and challenges of integrating computational intelligence with experimental chemistry.

Keywords: *Artificial Intelligence; Machine Learning; Chemical Synthesis; Retrosynthesis; Self-Driving Laboratories; Reaction Optimization; Large Language Models*

Introduction

Chemical synthesis underpins pharmaceuticals, materials science, and energy technologies. Traditionally, chemists have relied on experience-based heuristics and time-consuming experiments to design viable synthetic routes. The emergence of AI has introduced predictive accuracy and automation that outperform conventional methods in both speed and scope [1]. Modern AI systems leverage large reaction databases such as Reaxys, PubChem, and USPTO to train models capable of reasoning over millions of transformations, enabling automated synthesis planning, yield prediction, and optimization [2]. Recent work integrating large language models with chemistry tools has further expanded AI's ability to assist in scientific reasoning and workflow automation [3].

AI Approaches in Chemical Synthesis

1. Retrosynthetic Planning and Route Design

AI-based retrosynthesis systems can design synthetic routes backward from the target molecule, identifying feasible intermediates and reagents. Updated models such as AiZynthFinder 4.0 now utilize transformer and graph-based architectures to generate multi-step synthesis plans with improved interpretability [4]. Similarly, IBM's RXN platform employs language-model-based reasoning to translate chemical reactions into text representations, allowing computers to learn chemical reactivity [5].

2. Reaction Prediction and Yield Optimization

Predicting whether a reaction will proceed and at what yield is another area revolutionized by AI. GNNs trained on large reaction datasets can predict outcomes with remarkable accuracy. Pre-trained molecular models fine-tuned for yield prediction have reduced the experimental burden by identifying promising conditions early [2]. Bayesian optimization and reinforcement learning are increasingly applied to explore reaction parameters efficiently, accelerating reaction screening [1].

3. Generative Molecular and Reaction Design

Generative AI has emerged as a tool for proposing novel molecules and synthetic pathways. Recent invertible GNN-based frameworks not only design compounds with desired properties but also consider synthetic accessibility [6]. Large language model driven chemistry agents such as ChemCrow integrate reasoning, tool use, and data retrieval to propose synthesis strategies and analyze reactions, marking a shift toward foundation-model-based chemical discovery [3]. By integrating property prediction with retrosynthetic feasibility, AI can propose synthesizable molecules, bridging the gap between computational design and experimental realization [7].

4. Self-Driving and Automated Laboratories

AI integration with robotics has led to the rise of self-driving laboratories (SDLs) closed-loop systems that autonomously design, perform, and analyze experiments.

These platforms continuously learn from data to refine subsequent experiments, significantly accelerating discovery cycles [1,8]. Emerging autonomous research platforms such as AutoSciLab demonstrate interpretable scientific discovery through active learning and automated experimentation, highlighting the future of AI-driven laboratories [9].

Applications Across the Chemical Domain

Pharmaceutical Discovery: AI-assisted retrosynthesis and yield prediction help chemists identify efficient synthetic routes for drug candidates, minimizing development time and cost [4].
Catalyst and Reaction Optimization: Active learning and Bayesian optimization identify reaction parameters that maximize yield, selectivity, and sustainability [1].
Sustainable and Green Chemistry: Computer-aided retrosynthesis incorporates green metrics to minimize environmental impact by selecting safer reagents and reducing steps [10].
Materials and Energy Research: AI-driven synthesis has been applied in developing novel catalysts, batteries, and polymer materials [8].

Benefits and Impacts

Speed and Efficiency: Automated AI workflows accelerate experimental cycles and reduce human labor.
Resource Optimization: Predictive analytics minimize reagent consumption and energy waste.
Scalability: AI enables exploration of vast chemical spaces beyond human intuition.
Sustainability: Route selection guided by environmental impact contributes to green chemistry principles [10].

Challenges and Limitations

Despite its promise, AI-driven synthesis faces key challenges. Data quality remains a major limitation, as models rely on large, high-quality reaction datasets that are often incomplete or inconsistent [7]. Model interpretability and reliability issues persist, especially with deep learning and LLM-based systems, where plausibility may not always equal chemical validity [11]. Integration with experimental labs also requires robust automation infrastructure [8]. Ethical and safety considerations must be addressed to ensure transparent decision-making in autonomous platforms.

Future Perspectives

The near future will likely see full integration of AI models with automated experimentation, creating autonomous chemistry ecosystems. Cross-disciplinary collaboration between data scientists, chemists, and engineers will be essential [7]. Emerging foundation models such as ChemLLM and ChemDFM highlight the transition toward general-purpose AI systems capable of reasoning across diverse chemical tasks [12,13]. Quantum computing and community-driven data sharing initiatives may further enhance reaction prediction accuracy and reproducibility [5].

Conclusion

AI is no longer a theoretical tool but a transformative partner in modern chemical synthesis. From predictive retrosynthesis to autonomous experimentation and LLM-driven reasoning, AI empowers chemists to innovate faster, safer, and more sustainably. As data accessibility, interpretability, and automation advance, the fusion of AI and chemistry promises to redefine how molecules are discovered, designed, and manufactured.

Acknowledgment

I would like to express my sincere gratitude to all those who have contributed to the successful completion of this study titled "Integrating Artificial Intelligence into Chemical Synthesis: Advances, Applications, and Challenges."
First and foremost, I extend my heartfelt thanks to my project guide for their invaluable guidance, constant encouragement, and insightful suggestions throughout the research process. Their expertise has been instrumental in shaping this study.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| *Volume-3 Issue-1(I)* | *February-2026* | *ISSN: 3066-0637* | *Website:* https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030103

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465136

DOI Link:
https://doi.org/10.5281/zenodo.19465136

Volume: 3

Issue: 1(I)

Pp. 16-20

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 10 Jan. 2026

Revised: 20 Jan. 2026

Accepted: 03 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
A. Dayanand, Rao, D. V., R. Lavanya, K. Thirupathaih, A. Vasantha, & N. Deepika. (2026). DNA Interaction Profile of Newly Synthesized Ru (II) Complexes: Implications for Antimicrobial and Anti proliferative Activity. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 16–20. https://doi.org/10.5281/zenodo.19465136

DNA Interaction Profile of Newly Synthesized Ru (II) Complexes: Implications for Antimicrobial and Anti proliferative Activity

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Abstract

Ruthenium (II) complexes have emerged as promising candidates in medicinal inorganic chemistry due to their diverse coordination chemistry, photochemical activity, and potential therapeutic properties. In this study we synthesized two Ruthenium polypyridyl complexes with BMPIP ligand. The DNA binding interactions, photocleavage efficiency, and anticancer potential of a series of synthesized ruthenium complexes bearing polypyridyl and ancillary ligands. Spectroscopic and viscosity measurements indicate strong intercalative binding mode toward calf thymus DNA. Upon photoirradiation, the complexes exhibit significant pBR 322 DNA cleavage activity, attributed to the generation of reactive oxygen species and photoinduced electron transfer. Cytotoxic assays against selected human cancer cell lines reveal potent antiproliferative effects, comparable with to conventional chemotherapeutic agents, with minimal effects on normal cells. These findings highlight the multifunctional nature of ruthenium complexes as photo responsive anticancer drugs.

Keywords: *Ruthenium (II) complexes, BMPIP, pBR 322 DNA, CT-DNA DNA binding, antimicrobial activity, anticancer agents, metal-based therapeutics.*

Introduction

Metal-based therapeutics have become increasingly important in medicinal chemistry due to their structural diversity and unique biological mechanisms [1,10]. Among transition metals, ruthenium has emerged as a promising candidate for drug development because of its favourable kinetics, redox properties, and relatively low toxicity [2,11]. Several Ru (II) complexes have demonstrated strong anticancer and antimicrobial activity, particularly when coordinated with aromatic or heterocyclic ligands [3,12].

DNA remains one of the primary intracellular targets for therapeutic metal complexes. Binding interactions such as intercalation, groove binding, and electrostatic interactions can disrupt DNA replication and transcription processes, leading to inhibition of microbial growth and cancer cell proliferation [4,5,13]. Polypyridyl Ru (II) complexes are especially effective DNA binders due to their planar structures and ability to form π–π stacking interactions with nucleic acid bases [6,14].

Ruthenium (II) complexes have attracted increasing attention due to their versatile coordination chemistry and potential therapeutic applications [1,2]. In the present study, newly synthesized Ru (II) complexes were evaluated for DNA-binding properties and their antimicrobial and antiproliferative activity. Spectroscopic analysis, viscosity measurements, and molecular docking were employed to determine binding mechanisms, while antimicrobial and cytotoxic assays assessed biological efficacy. The complexes demonstrated strong DNA affinity through intercalative and groove-binding modes, consistent with previously reported polypyridyl ruthenium complexes [3–6, 15]

Biological evaluation revealed significant antibacterial activity and dose-dependent inhibition of cancer cell proliferation [7–9]. The results highlight the importance of ligand design in controlling DNA interactions and biological performance, supporting the development of multifunctional Ru (II)-based therapeutic agents [10–12]. Despite these advances, the relationship between DNA-binding behaviour and biological activity requires further investigation. Therefore, this study aims to synthesize new Ru (II) complexes, characterize their DNA interaction profiles, and correlate these findings with antimicrobial and antiproliferative activity.

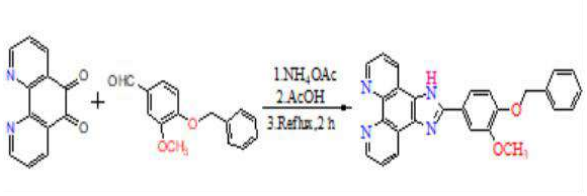
Synthesis

Synthesis of ligand 2-(3-methoxy-4phenoxyphenyl)-1-H-imidazo [4,5 f] [1,10] phenanthroline (BMPIP)

A mixture of phendione (1 mmol) and 4(benzyloxy)3-methoxybenzaldehyde (1.5 mmol), ammonium acetate and glacial acetic acid was refluxed with stirring for 2h. The solution was cooled and diluted with 25 mL of water. It was neutralised by drop wise addition of concentrated aqueous ammonia.

The precipitate was collected and purified by column chromatography on silica gel (60-100 mesh) with ethanol as eluent to yield golden yellow needles of BMPIP, which was suctioned filtered and recrystallised. (Fig. 2.1.) Analytical Data: C26H18N4O2 Calcd.(%): C:74.63; H: 4.34; N: 13.39; Found (%): C: 73.98; H: 4.28; N: 12.99; ESI-MS(m/z): 418. 1H NMR (DMSO-d6, 400M Hz; TMS, δppm): 8.92681(d, 2H), 7.85505 (d, 2H), 7.49900 (d, 1H), 7.43150 (t, 2H), 7.39470 (t, 2H), 7.34893 (d,1H), 7.21134 (d, 2H), 7.19002 (d, 1H), 5.59111(s,1H).

Analytical Data: $C_{26}H_{18}N_4O_2$ Calcd.(%): C:74.63; H: 4.34; N: 13.39; Found (%): C: 73.98; H: 4.28; N: 12.99; ESI-MS(m/z): 418. ^{1}H NMR (DMSO-d_6, 400M Hz; TMS, δppm): 8.92681(d, 2H), 7.85505 (d, 2H), 7.49900 (d, 1H), 7.43150 (t, 2H), 7.39470 (t, 2H), 7.34893 (d,1H), 7.21134 (d, 2H), 7.19002 (d, 1H), 5.59111(s,1H).



Synthesis of BMPIP

Synthesis of [Ru(bpy)$_2$BMPIP] $(ClO_4)_2$ $2H_2O$ (1)

This complex [Ru(bpy)$_2$BMPIP] $(ClO_4)_2$ $2H_2O$ is prepared by the similar procedure described for the above complex with a mixture of cis-[Ru(bpy)$_2$Cl$_2$].$2H_2O$ (0.5m mol) and BMPIP (0.5m mol).

Analytical Data: $RuC_{46}H_{38}Cl_2N_8O_{12}$ Calcd. (%) C, 51.79; H, 3.59; N, 10.50; Found (%):C, 50.63; H, 2.83; N, 9.68; ESI-MS(m/z): 1066. ^{1}H NMR (DMSO-d_6, 400MHz; TMS, δ-ppm): 8.886(d,2H), 8.8508(d,4H), 8.5306(d,4H), 8.0521(d,2H), 7.8840(t,4H),), 7.6157(t,4H), 7.593(t,2H), 7.4241(d,2H), 7.4053(t,1H), 7.3725(d,1H), 7.3576(d,1H), 7.3406(d,1H). ^{13}C-NMR (DMSO-d_6, 400MHz; δ-ppm): 157, 152, 150, 139, 138, 129, 71, 70.424, 56.336, 40.568, 40.360, 40.151, 39.943, 39.734, 39.526, 39.315.

Synthesis of [Ru(dmb)$_2$BMPIP] $(ClO_4)_2$ $2H_2O$ (2)

This complex [Ru(dmb)$_2$BMPIP] $(ClO_4)_2$ $2H_2O$ is prepared by the similar procedure described for the above complex with a mixture of cis-[Ru(dmb)$_2$Cl$_2$].$2H_2O$ (0.5mmol) and BMPIP (0.5mmol).

Analytical Data: $RuC_{50}H_{46}Cl_2N_8O_{12}$ Calcd. (%) C, 53.48; H, 4.13; N, 9.98; Found (%):C, 52.63; H, 3.78; N, 8.54; ESI-MS(m/z): 1122.8. ^{1}H NMR (DMSO-d_6, 400MHz; TMS, δ-ppm): 9.04058, 8.71482, 8.4, 8.04936, 7.89818, 7.4136, 7.16193. ^{13}C-NMR (DMSO-d_6, 400MHz; δ-ppm): 9.04058, 8.71482, 8.4, 8.04936, 7.89818, 7.4136, 7.1619

Physical Measurements

All the synthesized compounds are characterized by elemental analysis, mass, infrared, electron absorption and nuclear magnetic resonance spectroscopic methods. UV-Visible, Electronic Absorption spectroscopy recorded with an Elico BL 198 spectrophotometer. Fluorescence emission spectroscopic performed on an Elico SL 174 spectro fluorimeter, FTIR spectra were recorded on KBr disks on a Perkin–Elmer FT-IR-1605 spectrometer. Microanalyses (C, H, and N) were carried out with a Perkin-Elmer 240 elemental analyzer. ESI-MS in DMSO recorded on a LQC system (Finnigan MAT, USA) using CH_3CN as mobile phase. Nuclear Magnetic Resonance spectra ^{1}HNMR and ^{13}C [^{1}H] NMR) were recorded on a Bruker 400 MHz spectrometer with DMSO-d_6 as solvent at room temperature and tetra methyl silane (TMS) as the internal standard. Viscosity experiments were carried out on Ostwald Viscometer. Gel electrophoresis was photographed in Gel doc system (Alpha InfoTech Corporation). Thermo Scientific Multi Skan EX Elisa reader was used for MTT assay.

DNA Binding Experiments

Electronic absorption and Fluorescence titrations

Electronic absorption titrations and emission titrations of two complexes were monitored both in the absence and presence of CT DNA. The absorption titrations of the complex in tris-buffer were performed by titrating fixed concentration of complex, to which increments of the DNA stock solution were added. Complex–DNA solutions were allowed to incubate for 5 min before recording the absorption spectra or emission spectra. To evaluate the binding strength of the complex, the intrinsic binding constant Kb, with CT–DNA was obtained by monitoring the change in the absorbance at metal to ligand charge transfer (MLCT) band, with increasing concentration of DNA. The intrinsic binding constant Kb, of the Ru (II) complexes bound to DNA was calculated from Equation [21].

$[DNA]/(\varepsilon_a - \varepsilon_f) = [DNA]/(\varepsilon_b - \varepsilon_f) + 1/K_b(\varepsilon_b - \varepsilon_f)$

where [DNA] is the concentration of DNA. The apparent extinction coefficient (ε_a) was obtained by calculating Aobs / [Ru]. The terms ε_f and ε_b correspond to the extinction coefficients of free (unbound) and the

fully bound complex respectively. From plot of [DNA]/ ($\varepsilon_a - \varepsilon_f$) against [DNA] will give a slope 1/ ($\varepsilon_a - \varepsilon_f$) and an intercept $1/K_b(\varepsilon_b - \varepsilon_f)$. K_b is the ratio of the slope to the intercept.

In fluoroscence titrations the fraction of the ligand bound was calculated from the relation [22] $C_b = C_t [(F - F_0)/(F_{max} - F_0)]$, where Ct is the total complex concentration, F is the observed fluorescence emission intensity at a given DNA concentration, F_0 is the intensity in the absence of DNA, and Fmax is when complex is fully bound to DNA. Binding constant (K_b) was obtained from a Scatchard plot of r/Cf against r, where r is the C_b/[DNA] and C_f is the concentration of free complex.

Viscometric Titrations

Viscosity experiments were carried out with an Ostwald viscometer, placed in a thermostatic water bath to maintain at a constant temperature 30.0 ± 0.1 °C. Calf thymus DNA samples approximately 200 base pairs were prepared by sonicating in order to minimize complexities arising from DNA flexibility. Flow time was measured with a digital stopwatch, and each sample was measured three times, and then an average flow time was calculated. Data were presented as $(\eta/\eta_0)^{1/3}$ versus the [complex]/[DNA], where η is the viscosity of DNA in presence of complex and η_0 is the viscosity of DNA alone. Viscosity values were calculated from the observed flow time of DNA-containing solutions (t>100 s) corrected for the flow time of the buffer alone (t_0) [22, 23].

DNA photocleavage and agarose gel electrophoresis

For the gel electrophoresis experiments pH 8.0 buffer of 40 mM Tris base, 20 mM acetic acid, and 1 mM EDTA were used. A buffer of 10 mM Tris–HCland 1 mM Na_2EDTA was used for dilution of pBR322 DNA. Supercoiled pBR322 DNA (0.1 g/μL) was treated with ruthenium (II) complexes with concentrations of 20–60 μM, and the mixtures were irradiated at room temperature with a UV lamp (365 nm, 10 W) for 60 min. A loading buffer containing 25 % bromophenol blue, 0.25 % xylene cyanol, and 30 % glycerol (2 μL) was added. The samples were then analyzed by 0.8 % agarose gel electrophoresis at 50 V for 2 h. The gel was stained with 2 μL (from 1 mg/100 μL) ethidium bromide [24] and photographed under UV light. The gels were viewed with a gel documentation system and photographed using a CCD

Biological activity:

Complexes in the concentration range of 1–100 μM, dissolved in DMSO were added to the wells. Control wells were prepared by addition of culture medium (200 μL). The plates were incubated at 37 °C in a 5% CO2 incubator for 48 h. After 48 h incubation, stock MTT dye solution about 20 μL was added to each well and the plates were wrapped in aluminium foil and incubated for 4 h at 37 °C. The purple formazan product was dissolved by the addition of 100 μL of 100 % DMSO to each well. The absorbance was monitored at 620 nm using a 96-well plate reader. A well containing culture medium without cells were used as a negative control and cisplatin was used as a positive control. DMSO was used as the vehicle control. A stock solution of cisplatin (10 mM in DMSO) was freshly prepared for every experiment. The stock solutions of the metal complexes were prepared in DMSO. Data were collected for three replicates each to obtain the mean values. The IC_{50} values were determined by plotting the percentage viability verses concentrations on a logarithmic graph and reading the concentration at which 50 % of cells remained viable relative to the control. HeLa (human cervical cancer cell line) were used for this study.

Characterization of Complexes

The percentage of elements like carbon, nitrogen and hydrogen (analysis of C, N and H) in complexes by elemental analysis are determined. E As expected, this elemental analysis is in good agreement with the calculated values, within the limits of experimental errors.

Spectroscopic characterization confirmed successful coordination between ruthenium ions and ligands, resulting in stable octahedral complexes. Similar structural features have been reported in previously synthesized bioactive Ru (II) complexes [3,15].

DNA Interaction Studies

UV–visible spectroscopy revealed hypochromic effects and bathochromic shifts upon DNA addition, indicating strong interaction between complexes and DNA [4,5]. Fluorescence quenching experiments suggested intercalative binding, while viscosity measurements supported insertion of complexes between DNA base pairs [6,16]. UV–visible spectroscopy revealed hypochromic effects and bathochromic shifts upon DNA addition, indicating strong interaction between complexes and DNA [4,5]. Absorption spectrum of ligand BMPIP shown peak at 330 nm which corresponds to transition of ligands. The absorption spectrum of complexes 1&2 shown peak at 360 nm which corresponds to transition of ligands and another peak at around 460nm due to MLCT metal to ligand charge transfer absorption peak, these complexes exhibited hypochromism of 26.6% and 24.7% respectively at the MLCT band that suggests the formation of complexes, the intrinsic binding constants K_b were determined by monitoring the changes of absorbance in the MLCT band as 4.13x105 and 3.88x105 for complexes 1 and 2 respectively. Fluorescence quenching experiments suggested intercalative binding, the complex emits prominent luminescence in Tris-buffer with a maximum emission wavelength of about 650 nm. The well-behaved titration of the complex with CT-DNA is displayed in Fig 3.2.(b) shows fluorescence spectrum of complexes 1 with addition of CT–DNA, in Tris buffer with increasing concentration of CT-DNA. The arrow shows the fluorescence intensity change upon increase of DNA concentration. Inset: Scatchard plot of r/Cf vs r. while viscosity measurements supported insertion of complexes between DNA base pairs, the relative viscosity increased steadily as expected with the intercalation mode of binding [6,16]. In classical intercalation, the DNA helix lengthens as base pairs are separated to accommodate the bound ligand leading to an increase in the viscosity of the DNA solution

[21]. In the relative viscosities of complexes 1&2 are compared with the relative viscosity of well-known intercalator ethidium bromide.
The order of relative viscosity of the two complexes is as follows EtBr > [Ru(bpy)2BMPIP]2+>[Ru(dmb)2BMPIP]2+

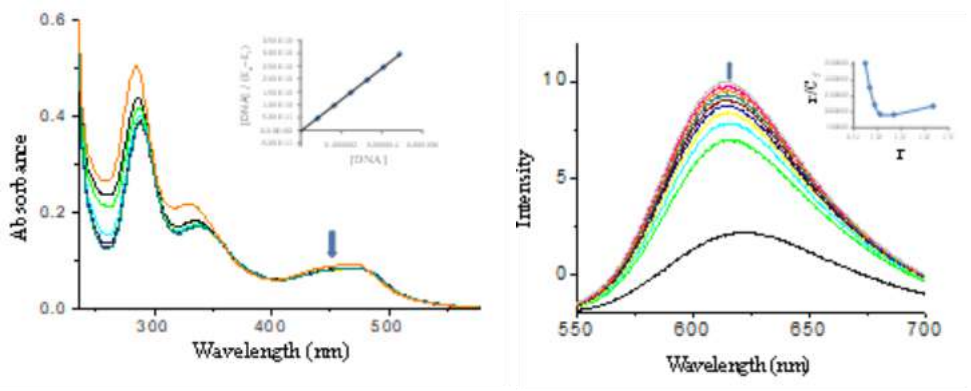


Fig. 3.2.(a) Absorption spectrum of $[Ru(phen)_2(BMPIP)]^{2+}$ (1) in tris-buffer upon addition of CT–DNA in absence and presence of CT–DNA, the [complex] = 10–15 μM; [DNA] = 0–126 μM. Insert plots of $[DNA]/(\varepsilon_a - \varepsilon_f)$ vs [DNA] for the titration of DNA with complex. Arrow shows change in absorption with increasing DNA concentration.
Fig 3.2(b) The fluorescence spectrum of $[Ru(phen)_2BMPIP]^{2+}$(1) with addition of CT–DNA, in Tris buffer with increasing concentration of CT-DNA. The arrow shows the fluorescence intensity change upon increase of DNA concentration. Inset: Scatchard plot of r/C_f vs r.

Photoactivated cleavage studies

Both complexes with circular plasmid DNA are subjected to electrophoresis, Fig. 3.3 shows the gel electrophoresis separation of pBR322 DNA after incubation with various concentrations of both complexes and irradiation at 365 nm for 60 min. No obvious DNA cleavage was observed in control in which complex was absent. With the increasing concentration of all the four complexes, the amount of form I was diminished gradually, whereas that of form II was increased. Furthermore, the cleavage effect was found to be concentration dependent. Under the comparable experimental conditions both complexes exhibited efficient DNA photo cleavage activity, which supports their binding affinity towards DNA as shown in Fig: 3.3

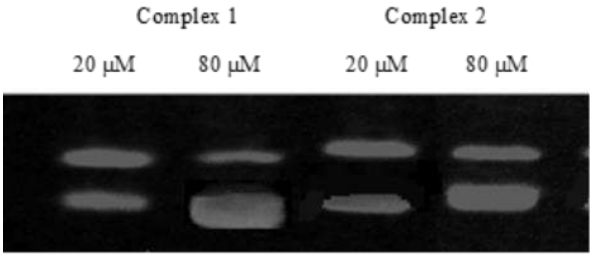


Fig: 3.3 The pBR 322 DNA photocleavage of complex 1 and complex 2

In vitro cytotoxicity assay

The cytotoxicity of all complexes against HeLa cell lines was evaluated by MTT assay. Similar cytotoxicity assays are commonly used to evaluate the therapeutic potential of metal-based anticancer compounds [8,12,18]. Cisplatin and DMSO used as positive and negative controls, respectively. After treatment of HeLa cell line for 48 h with both complexes in the range of concentrations (4-100μM). The inhibitory percentage against growth of cancer cells was determined. The cytotoxicity of complexes was found to be concentration dependent. The cell viability decreased with increasing the concentrations of complexes IC50 values of complexes 1 and 2 and cisplatin are 41.34±0.5 μM, 48.320.5 μM and 4.8±0.5 μM respectively.

Anti-microbial studies

Antimicrobial activity was assessed using Agar Well Diffusion Method against Gram-positive and Gram-negative bacterial strains. Bacillus subtilis, Staphylococcus aureus and Escherichia coli. Penicillin and Streptomycin are taken as standards under identical conditions for comparison. The minimum inhibitory concentrations (MIC) of the complexes 1and 2 given in Table 3.5. The experimental results of antibacterial activity indicated a variable degree of efficacy of the compounds against different strains of bacteria

Table: The MIC values of the complexes 1and 2.

MIC (µg/ml)			
Complexes	*B.Subtilis*	*S.aureus*	*E.coli*
Complex 1	25	31	34.2
Complex 2	45	40	55
Penicillin	1.562	1.562	12.5
Streptomycin	6.25	6.25	6.25

Conclusion

The main theme of this work is to do comparative study of the DNA binding and cleavage studies of Ruthenium polypyridyl complex with different ancillary ligands. Newly synthesized Ru (II) complexes demonstrated strong DNA-binding properties and significant antimicrobial and antiproliferative activity. Intercalative binding mechanism contributed to biological effects. The binding strength and biological activity of complex 1 is greater than complex 2, due to steric hindrance of complex 2, which attributed to the methyl groups present on ancillary ligand dmb. Cytotoxicity assays in vitro showed that two complexes have antitumor activity but less than cisplatin, complex (1) displays higher antitumor activity than complex (2). The study underscores the potential of rational ligand design in developing multifunctional ruthenium-based therapeutics. Future studies should include in vivo evaluation, pharmacokinetic studies, and toxicity assessment to further validate clinical potential [11,19,20].

Acknowledgment

I would like to express my sincere gratitude to all those who have contributed to the successful completion of this research work titled "DNA Interaction Profile of Newly Synthesized Ru (II) Complexes: Implications for Antimicrobial and Antiproliferative Activity."

First and foremost, I am deeply indebted to my project guide for their invaluable guidance, continuous encouragement, and insightful suggestions throughout the course of this research. Their expertise and mentorship have played a vital role in the successful completion of this study.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030104

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465226

DOI Link:
https://doi.org/10.5281/zenodo.19465226

Volume: 3

Issue: 1(I)

Pp. 21-29

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 10 Jan. 2026

Revised: 20 Jan. 2026

Accepted: 03 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Rao, M. N. (2026). Microplastic Pollution in Aquatic Ecosystems: A Comprehensive Review of Environmental Impacts and Potential Solutions. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 21–29.
https://doi.org/10.5281/zenodo.19465226

Microplastic Pollution in Aquatic Ecosystems: A Comprehensive Review of Environmental Impacts and Potential Solutions

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Abstract

Microplastics, defined as plastic particles that measure less than 5 mm, are currently pervasive contaminants in aquatic environments, attributed to the increasing global production of plastic and the environmental fragmentation of bigger plastic items. This thorough overview brings together what we know about microplastic sources, where they are found, how they affect the environment and health, how to study them, how to reduce them, and where future research should go. Microbeads and fibers from synthetic textiles are examples of primary microplastics. Secondary microplastics, on the other hand, come from the breakdown of macroplastics through environmental weathering. Globally, and especially in India, microplastic pollution is a persistent problem in freshwater and marine habitats. This is due to things like wastewater treatment facilities, fishing, urban runoff, and incorrect disposal. The effects can be physical harm and changes in behavior in aquatic species, as well as the transfer of hazardous contaminants via the food chain, which threatens ecological stability and human health through seafood intake. Improvements in sampling and spectroscopic identification make it easier to find things, but they also have problems with standardization and contamination. Mitigation via upstream source reduction, enhanced waste management, biodegradable materials, regulatory frameworks, and public involvement demonstrates potential but necessitates scaling and enforcement. Some important areas of research that need more work are the long-term consequences of nanoplastics, the effects on the environment over time, and the need for standardization of analytical methods. To protect public health and aquatic biodiversity, we need to work together across disciplines and regions to deal with microplastic pollution.

Keywords: *Microplastics (MP), Aquatic environments, Marine habitats, Ecological stability, Mitigation, Nanoplastics, Analytical methods, Aquatic biodiversity.*

Introduction

Microplastics and Their Sources:

Microplastics are plastic particles that are less than 5 mm in diameter.[1,2] They can be made directly from small plastics (primary microplastics, like microbeads and pre-production pellets) or by breaking up larger plastic debris (secondary microplastics) through environmental processes like photooxidation, mechanical abrasion, or biological degradation.[1–3]

Overview of the Global Plastic Pollution Crisis

Scale of Global Plastic Pollution

The global plastic pollution crisis is a huge environmental problem that is mostly caused by the material's characteristics and the huge increase in production since the middle of the 20th century.

Explosion in Production: Since the middle of the 20th century, the amount of plastic made around the world has grown by a huge amount.[3–5]

Annual Ocean Input: This production creates a huge amount of pollution, with more than 8 million tons of microplastic debris coming from land sources into the oceans every year.[6]

Ubiquity: Plastics are everywhere because they are cheap, strong, and don't break down easily. They are currently found in almost all major bodies of water, such as freshwater, marine, and even karst groundwater.[3,6]

Importance of Studying Microplastic Contamination in Aquatic Environments

It is very important to focus on aquatic ecosystems since microplastic pollution is a big threat to the important ecological functions that these systems supply.

Essential Ecosystem Functions: Aquatic ecosystems are essential for biodiversity, supporting marine life, facilitating primary productivity (the foundation of the food web), and enabling global nutrient cycles.[7]

Magnified Ecological Impact (Carrier Effect): Microplastics are a double hazard because they can carry other pollutants, like heavy metals and persistent organic pollutants (POPs).[7,8]

Hazard to Health: Microplastics transport these toxins and mess with biological processes, which makes their ecological impact even bigger across the food web. In the end, this is a hazard to humans because they can be eaten.[9]

Objectives of the Review

The review's main goal, as clearly mentioned in the publication, is to give a full summary of what we now know about microplastics in aquatic systems. The review does this by carefully looking at recent scientific studies in six important areas:

Sources: Finding the main and secondary sources of microplastics.

Distribution: Charting the occurrence of microplastics in several aquatic ecosystems.

Ecological impacts: Effects on the organism, keystone species, and community structure

Analytical Methods: Looking at the methods that are currently employed for sampling, separating, and characterizing.

Mitigation Strategies: Describing the essential ways to cut down on sources, handle waste, and make policy changes.

Future Research Directions: Emphasizing the significant deficiencies in existing knowledge, including the destiny of nanoplastics and the necessity for prolonged ecological investigations.

In summary, the review is a fundamental scientific resource that helps us comprehend the widespread microplastic pollution by linking its basic qualities to the steps that need to be taken to deal with the problem and future study.

Sources and Distribution of Microplastics in Aquatic Environments

Microplastics: Primary vs. Secondary

Primary microplastics are tiny particles made for use in cosmetics, personal care items, and industrial processes. Examples include microbeads, nurdles, and microfibers from textiles. Secondary microplastics are pieces that break off of bigger plastics because of UV light, weathering, or microbes (for example, broken bottles and bags).[1–3]

Key Sources

Industrial and Sewage Runoff: Even while wastewater treatment plants remove a lot of waste, they nevertheless send a lot of microplastic fibers and beads into bodies of water.

Microplastic fibers (MPFs) have become a persistent and prevalent category of pollutants introduced into aquatic ecosystems, with wastewater treatment plants (WWTPs) serving as both essential interception locations and significant conduits for their environmental distribution. Recent studies have shown that WWTPs are usually quite good at removing microplastics, with rates of about 99%. Even while WWTPs do a great job, they nevertheless release a lot of waste since they process a lot of waste water every day. Even the ~1% of microplastics that don't get caught in the treatment process can mean millions of fibers getting into bodies of water every day.[10,11]

Quantitative evaluations consistently indicate that polyester is the most commonly identified polymer in wastewater streams, primarily resulting from the laundering of synthetic textiles. The research emphasizes that microplastic fiber concentrations in influent can attain thousands of fibers per liter, and while tertiary treatments such sand filtration can improve removal rates by as much as 98%, they do not completely remove MPFs from the effluent.[10–12]

The examined literature emphasizes the significance of uniform sampling and analytical methodologies. The recommended techniques involve taking grab samples of 1–2 liters of wastewater, breaking down organic debris with 30% hydrogen peroxide at 100°C, and utilizing glass fiber or alumina oxide membranes with pore diameters below 20 µm to separate microplastics. Microscopic enumeration combined with µFTIR spectroscopy continues to be the benchmark for fiber quantification and polymer identification. These methodological discoveries underscore the want for cohesive analytical frameworks to guarantee dependable, comparable datasets across investigations.[12–14]

The analyzed findings clearly show that WWTPs are good at stopping microplastic pollution, but their existing treatment technologies can't completely stop MPF release because of the high volume of throughput. This continual discharge shows that we need to quickly improve tertiary treatment methods, make better upstream textile designs, and make sure that standardized MPF monitoring techniques are followed to lessen the environmental impact of microplastic fibers.[12–15]

Navigation/Fishing/Aquaculture: Fishing nets and ropes, especially those made of low-density polyethylene (LDPE), let out a lot of fibers. Ship operations also add to the trash.[16,17]

Fishing gear, notably nets and ropes made of low-density polyethylene (LDPE), is known to be a major cause of marine microplastic contamination. LDPE is good for marine use since it floats, resists chemicals, and is strong enough to last a long time in the water. The attached document's quantitative degradation assessments show that LDPE that is exposed to marine environments breaks down physically and chemically in ways that can be measured, which directly leads to more microplastic fibers being released.[17]

Experimental weathering tests show that LDPE loses mass over time when exposed to UV light and seawater. Studies have shown that mass loss can be as high as 1.2–1.45% over long periods of age. These losses are due to the breaking of surface layers, fractures, and polymer pieces. FTIR spectroscopic assessments demonstrate enhanced oxidation via elevated carbonyl peak ratios, substantiating that photo-oxidation expedites polymer embrittlement and fragmentation.[14,17]

Microscopy-based surface morphology analyses reveal that LDPE forms deep grooves, pits, and crack networks upon weathering, resulting in quantifiable increases in surface roughness that correspond with the initial stages of microplastic shedding. Old LDPE, in particular, has big changes in contact angle values, which means that its hydrophobicity has gone down because of oxidation and chain scission. These alterations to the surface are measurable signs of how likely it is that microplastics will be released.[17,18]

Fishing operations make this worse. Everyday tasks like trawling, hauling, dragging, and handling on deck put LDPE gear through frictional stresses that make it break apart more. The paper says that fishing nets and ropes get a lot of mechanical wear and tear, and that the diameter of LDPE rope fibers gets smaller after several cycles of wear and tear. This mechanical thinning is directly linked to the micro fibre coming off.[17]

Ship operations, such as mooring, anchor handling, and surface dragging, also cause wear and tear on the ship. The study says that wave-induced motion and mechanical contacts provide abrasion forces that speed up the wear of LDPE fibers. This leads to the gradual loss of material and the release of microplastic pieces.[17]

The quantitative degradation indicators—1–1.45% mass loss, carbonyl index rises, surface roughening, and observable fibre diameter reductions—show that LDPE fishing gear provides a constant, measurable source of microplastic fibres in normal maritime circumstances. The combination of environmental weathering and routine maritime operations makes it even more likely that LDPE fragments will keep breaking off. This shows that we need better polymer formulations, protective coatings, and other materials to reduce microplastic emissions from the fishing and shipping industries.[17–19]

Improper Disposal and Urban Runoff: Microplastics are more likely to be found in surface waters and sediments in cities, heavily inhabited areas, and when people litter directly.

Microplastic (MP) contamination of India's surface waters has reached alarming levels, with numerous studies measuring the amount, types of polymers, and other pollutants that are present at the same time. Recent studies have shown that a lot of MPs are found in rivers, lakes, and even groundwater all over India. These MPs come from broken-up plastic trash, industrial waste, sewage leaks, and bad waste management systems.[20]

The document's quantitative assessments show that there is a lot of variances in the space between freshwater bodies. For example, Red Hills Lake in Tamil Nadu has an average of 5.9 MP items/L of surface water, and sediments have an average of 27 items/kg, which shows that both water-column transit and benthic accumulation are happening. These MPs are constructed of HDPE, LDPE, and PP and come in the form of fibers, pieces, pellets, and films.[20,21]

Kerala's Veeranam Lake is even more polluted, with 28 MP items/km² in the surface water and 309 items/kg in the sediments. Most of the items are PE, PP, and PS fragments and films. Heavy metals like Cd, Cr, and Zn are found with the MPs, which shows that they are chemical stressors that work together.[20–22]

A lot of plastic comes from many different places into major Indian rivers. The Ganga and Yamuna transport MPs such beads, films, and fibers composed of polyacetylene, EVOH, and PVC. Heavy metals like Pb, Cd, and Fe were found along with the MPs, which made the ecological concerns even worse.[20,23]

MPs have also gotten into groundwater systems. Borewell samples from Tuticorin (Tamil Nadu) exhibited 4.2 MP items/L, with PET and PP as the predominant polymers, thereby validating that microplastic leakage extends beyond surface waters.[20,21]

The observed MP levels in major rivers throughout the world, like the Yangtze (500–3000 particles/m³), Rhine (20–7000 particles/m³), and Ganges (60–500 particles/m³), seem to be in line with the levels seen in India. This suggests that freshwater plastic loading is a global problem.[20,24]

The quantitative evidence collectively indicates that Indian water bodies possess elevated quantities of microplastics, frequently coupled by heavy metals and persistent organic contaminants. This dual contamination speeds up ecological hazards by trophic transmission, biomagnification, and chemical adsorption. The uploaded document says that these levels are likely to go rise if there isn't uniform monitoring, stronger wastewater treatment, and MP-specific regulatory frameworks. This would make India's surface water quality and ecosystem health even worse.[20]

Patterns of Distribution in Different Aquatic Ecosystems:

Microplastics are now known to be everywhere in aquatic ecosystems around the world, including lakes, rivers, estuaries, and polar and tropical zones. The density of their polymer kinds has a big effect on where they end up. For example, buoyant polymers like polyethylene (PE) and polypropylene (PP) often stay afloat or collect along shorelines, while denser materials like polyvinyl chloride (PVC) tend to sink and settle in sediments. Quantitative studies consistently demonstrate that regions adjacent to urban centers or areas of significant human activity display heightened microplastic concentrations in both freshwater and marine environments.[25,26]

When we look at different ecosystems, we see that freshwater bodies like the Yangtze River and Lake Victoria have a lot of microplastics in them. Most of these come from urban runoff and sewage, and they are mostly fibrous particles that range from 100 to 3,000 particles per cubic meter.[27] Microplastics tend to stay in sediments in wetlands like India's Sundarbans and the Mekong Delta, which means that benthic invertebrates have more of them than rivers do. Microplastics are found in marine areas including the Mediterranean and the Bay of Bengal, from surface waters to deep-sea sediments. There is evidence that trophic transfer affects fish and seabirds. Microplastics can also be found in polar ecosystems, as in sea ice, snow, and local animals. These microplastics come from global movement and atmospheric deposition.[25,26]

In India's cities, waterways like the Ganges carry a lot of microplastics because of runoff and industrial discharge. In certain places, there are concentrations of 4,000 to 13,000 particles per cubic meter. Research

underscores the significance of wetlands, estuaries, and areas characterized by intricate flow dynamics as repositories for microplastics and concomitant contaminants. The polymer density and hydrological circumstances create different patterns of microplastic pollution in India's many bodies of water.[22,23,25]

Quantitative analyses and conceptual models in the literature demonstrate the gradual accumulation of microplastics from surface water through sediments and their integration into aquatic food webs, transitioning from plankton and benthic invertebrates to higher trophic levels, including seabirds and marine mammals. Bar and line graphs show how being close to cities and factories is closely related to the amount of microplastics in the air. This shows how population density and local waste management techniques affect the amount of microplastics in the air. This study highlights the imperative to comprehend and regulate microplastic contamination through tailored solutions that take into account the distinct ecological and socio-economic circumstances of each ecosystem.[25]

Things that affect how microplastics are spread:

Microplastic dispersal in aquatic ecosystems is a multifaceted and evolving process controlled by an interplay of physical and anthropogenic forces. Water currents, wind, local hydrodynamic conditions, and meteorological events like storms are some of the main physical forces that affect how microplastics migrate and where they end up.[3,28,29] These pressures decide how microplastics move both horizontally over long distances and vertically through the water column. For example, ocean currents are the main way that microplastics move from coastal and land-based sources to the middle of the ocean, where they build up in areas like subtropical gyres. Wind is very important for vertical mixing. When the wind is strong, it moves buoyant plastics deeper into the water column, which lowers concentrations on the surface. Microplastics tend to build up in places with complicated water circulation, including estuaries and lagoons, where the currents are weaker and the sediments are more likely to interact with them.[3,30]

Severe weather events, especially storms, have a big effect on how microplastics spread because they quickly move them up and down and across the ground. Storms can move microplastics from land surfaces into rivers and coastal waters, resuspend sediment-bound particles, and move them offshore or to various depths. This generally leads to higher concentrations of microplastics in places along the coastline and at the mouths of rivers after storms. The variety in hydrodynamic conditions and the occasional disturbance caused by storms lead to large differences in the concentration of microplastics over time and space. This makes it harder to keep track of pollution patterns, but it also shows how important these physical processes are in shaping them.[3,31]

People's actions have a big impact on where microplastics end up, especially when it comes from places with a lot of people. Urban runoff, sewage discharge, and other human-made inputs release more microplastics into water bodies in coastal areas with high populations and industrial activity. This creates pollution hotspots near the coastline. In cities along the shore, concentrations can reach several thousand particles per cubic meter. In rural or distant locations, on the other hand, concentrations are usually much lower, generally only tens to hundreds of particles per cubic meter. The interaction between environmental forces and human activity determines the regional distribution of microplastics, underscoring the need for comprehensive strategies that incorporate both natural transport mechanisms and source inputs for effective pollution management and mitigation in marine and coastal ecosystems.[3,22]

Environmental Effects of Microplastic Pollution:

Microplastic contamination has a big effect on aquatic life in many ways, from physical harm to ecosystem-wide problems. Microplastics are eaten by many aquatic animals, such as zooplankton, fish, bivalves, mussels, marine mammals, and birds, since they are small and seem like natural food particles. Eating something can produce abrasions and blockages in the digestive track, which makes it hard to eat and digest. For instance, mussels and fish get tissue damage and obstructions in their guts that make it harder for them to eat and grow. In extreme instances, particularly among children or individuals with significant exposure, this may result in fatality. Research has recorded detrimental growth and survival rates in bivalves, larvae, and juvenile fish subjected to microplastics, measuring declines in growth rates and reproductive success attributed to compromised feeding efficiency.[2,5,16]

Microplastics not only have direct physical consequences, but they also let dangerous pollutants move through aquatic food webs and build up in living things. Lower trophic creatures that eat microplastics send them up the food chain to fish, seabirds, and mammals that eat them. Microplastics take in and hold onto heavy metals, antibiotics, endocrine disruptors, and persistent organic pollutants (POPs) from the environment. These toxins build up in living things and become more dangerous at higher trophic levels, which increases the risk of exposure. For example, the levels of mercury and polychlorinated biphenyls (PCBs) rise dramatically along food chains, which is very bad for the health of both predators and people who eat seafood. This pollutant transport associated with microplastics undermines ecological stability and has been directly correlated with health issues in human populations dependent on marine protein sources.[2,32,33]

Microplastic damage is made worse by physiological and behavioral effects. Exposure leads to oxidative stress by creating reactive oxygen species (ROS), which harm cells in algae, diatoms, and higher organisms. Photosynthetic efficiency diminishes in primary producers, and metabolic disturbances arise throughout trophic levels, shown in modified lipid metabolism in fish and compromised energy storage. Sex ratios that are not balanced and fertility consequences can cause immune reactions, problems with reproduction, and worse survival rates for offspring. In terms of behavior, creatures eat less, have trouble avoiding predators, migrate in strange ways, and modify how particles sink and stick together. These changes affect nutrient cycles and interactions in the ecosystem. Experiments on chronic exposure regularly show higher death rates and sublethal consequences, showing how

microplastics are a major threat to biodiversity, ecosystem processes, and ultimately, human health through environmental contamination and eating seafood.[2,34]

Microplastics have significant ecosystem-level effects, particularly on keystone species and filter feeders that are essential for preserving the structure and function of aquatic communities. Quantitative research substantiates this extensive impact across multiple significant populations. The copepod Neocalamus cristatus eats about one microplastic particle for every 34 of its kind, while the euphausiid Euphausia pacifica eats about one particle for every 17 of its kind. Mollusks, which are another important type of filter feeders, have measurable amounts of microplastics in them. For example, the blue mussel (Mytilus edulis) has roughly 0.27 ± 0.3 particles per gram of wet weight, and the Pacific oyster (Crassostrea gigas) has 0.47 ± 0.16 particles per gram. Arenicola marina, a kind of sediment feeder, similarly collects microplastics at a rate of about 2.8 particles per gram of wet weight. The damaged health and function of these keystone and foundational species can disrupt ecosystem dynamics by affecting food webs.[2,35,36]

Trophic transfer makes the effects of microplastics even worse since these particles travel from lower to higher trophic levels. For instance, sea turtles (Caretta caretta) have been found to eat trash, and 96.2% of the trash was plastic. This shows that there is a lot of contamination at the top levels. In bird species including the grey heron (Ardea cinerea), mute swan (Cygnus olor), and mallard (Anas platyrhynchos), researchers have found an average of 4.3 ± 2.6 particles per bird. Microplastic ingestion has been recorded in large mammals such as the humpback whale (Megaptera novaeangliae), with 16 plastic particles identified in a single specimen. These results give strong proof that microplastics are found in many parts of ecosystems and build up in animals that play important ecological roles.[2,37,38]

The main way that contaminated seafood and water can hurt people's health is through eating them. Quantitative studies indicate that fish, such as the blackmouth catshark (Galeus melastomus), accumulate approximately 0.34 ± 0.07 microplastic particles per individual, comparable to accumulation rates in economically significant shellfish like Mytilus edulis (0.27 ± 0.3 particles/g) and Crassostrea gigas (0.47 ± 0.16 particles/g). [39]There are health concerns linked to eating microplastics, both physical and chemical. For example, microplastics can obstruct the digestive system and cause inflammation. They can also carry harmful chemicals including PCBs, PAHs, and heavy metals. Microplastics are a worrying source of environmental contamination and dietary exposure since they can build up in living things and create health problems in people. Even if there aren't many concrete numbers regarding how risky microplastics are for people, a lot of studies and critical reviews show how important it is to deal with microplastic contamination to protect both public health and the environment.[2,40]

Methods for Detection and Characterization of Microplastics Using Analytical Methods:

Analytical techniques for identifying and describing microplastics in aquatic settings encompass several essential procedures customized to particular environmental conditions and study objectives.[41]

Techniques for Sampling: Depending on whether the aim is surface waters, sediments, or biota, sampling techniques must be changed. Common methods for sampling include net tows for surface water, sediment core collection, and grab sampling for sediments on the bottom. Dissection is done on biota to study how they eat microplastics. The size of the mesh in nets and the way the study is set up, on the other hand, have a big effect on the recovery rates of microplastics, which affects how accurate the detection is.[41,42]

Separation and Isolation: After being collected, the samples are put through processes to separate the microplastics from the other parts of the matrix. Using saline or hypersaline solutions for density separation takes use of the fact that polymers and sediments or biological materials float differently. Then, filtration makes plastic particles more concentrated for study. Chemical digestion breaks down organic substances in biotic samples to get rid of plastics.[41–43]

Identification and Quantification Techniques: For the first qualitative assessment of the shape, size, and color of microplastics, visual inspection and microscope are the main instruments used. Fourier Transform Infrared (FT-IR) spectroscopy and Raman spectroscopy are two common spectroscopic technologies used to definitively identify polymers and provide them a more complete description. These new approaches give molecular fingerprints that are important for sorting microplastics by polymer type. This makes identification more accurate than just looking at them.[14,44]

Problems and Limitations: Microplastic analytical methods are useful, but they have a lot of problems. There is no consistent agreement on how to classify microplastics by size or kind, which makes it hard to compare studies. The recovery rates differ a lot based on the procedure and the lab, and airborne contamination from fibers is always a danger for sample adulteration. Also, a lot of ways take a lot of time and work and need particular equipment, which makes it hard to increase throughput and scale. Ongoing research seeks to enhance in-situ detection technologies and standardize methodologies to augment efficiency and reliability in microplastic analysis.[45,46]

Strategies for reducing risk and their effects on policy:

Source Reduction: Since July 2022, India has banned single-use plastics, which has started to cut down on the amount of plastic garbage that people throw away, which is a big cause of microplastic pollution. However, enforcement is different in different parts of the country. For example, Delhi and Bengaluru have a lot of plastic garbage every day (1,113 and 6,000 tonnes, respectively), yet they don't have enough processing capacity. Also, microbeads are no longer allowed in cosmetics, which is in line with initiatives around the world to cut down on direct microplastic inputs. National programs like Swachh Bharat Abhiyan run public campaigns to create awareness and encourage people to use less plastic.[47,48]

Improvements in Waste Management: Only around 8% to 15% of India's 9.3 million tons of plastic waste per year is properly recycled. Nineteen percent of it is never collected and is commonly dumped or burned, which makes pollution and health problems worse. Investments are being made to improve recycling facilities and modernize wastewater treatment plants, especially in coastal and metropolitan areas where microplastic hotspots are common because of rivers and trash from fishing gear. But there are still big problems with separating garbage, collecting it efficiently, and covering all the facilities. These problems need to be solved by all the ministries and states working together.[49,50]

Innovation in biodegradable materials: India's low per capita plastic usage (11 kg/year, lower than the worldwide average) shows some restraint, yet the country is one of the biggest producers of plastic in the world. Researchers are looking into biodegradable options and building up local production capabilities to replace plastics that don't break down in packaging and farming. Adoption is still hampered by high costs and the difficulty of scaling up, but government incentives and partnerships between businesses are helping to start trial programs in this area.[50,51]
Policy and Governance: National policies like the Plastic Waste Management Rules (2016, updated 2022) set the rules, but enforcement and cooperation across agencies need to be better. The Central Pollution Control Board has been told to look into microplastics as part of the requirements for ambient air quality because they are bad for the environment and people's health. State-level programs and court actions, including those by the National Green Tribunal, are making people pay more attention and take action.[50,52]

Public Awareness and Education: Citizen science projects and public engagement efforts are becoming more popular in India. They give communities the tools they need to record and minimize plastic pollution. Coastal cleanups, educational outreach, and advocacy all help people take better care of the environment. However, changing people's behavior on a big scale is hard because cities are growing quickly and people from different backgrounds live there.[50]

India's efforts to reduce microplastic pollution are moving forward through a combination of rules, infrastructure, technology, and social change. However, it is still very important to deal with systemic problems in waste management, make biodegradable alternatives more widely available, and make sure that governance is consistent in order to lower the amount of microplastics in Indian habitats and protect public health and biodiversity. This synthesis focused on India shows how important it is to keep using integrated, context-sensitive techniques to deal with the growing problem of microplastic contamination.[49-52]

Future Research Directions:

Existing knowledge deficiencies in microplastic research provide significant obstacles to comprehensively understanding and addressing this widespread contaminant. Even while research has grown quickly over the last ten years, there are still several important areas that are not well understood. Tropical freshwater habitats, such as those prevalent in India, are significantly under-researched relative to marine systems, hindering comprehension of microplastic dynamics in these vital settings influenced by untreated wastewater, fluctuating flooding patterns, and several reservoirs. Also, we don't know much about the destiny, transport, toxicity, and biological effects of nano-sized plastics (nanoplastics), which makes it hard to figure out what they mean for the environment and health.

There isn't much research on long-term, in situ measurement of microplastic effects, which makes it hard to understand how they affect ecosystem stability, food web dynamics, and nutrient cycles over time. The health effects to humans from cumulative exposure to microplastics and their related adsorbed pollutants are little recognized due to fragmented and occasionally contradictory evidence. Also, the lack of common definitions, classifications, and analytical techniques makes it hard to compare data from different research and places. This diversity makes it harder to figure out what hazards are, how risky they are, and how to make policies around the world.

To surmount these obstacles, current and forthcoming research initiatives underscore the necessity for standardized, validated methodology, multidisciplinary long-term monitoring, and mechanistic investigations focusing on exposure pathways, toxicological mechanisms, and ecosystem-level repercussions. To make sure that regulations and mitigation programs work, we need to make progress in standardizing sampling, detection, and quantification procedures so that we can have reliable, comparable data. It is especially important to fill these gaps in understanding in places like India, where microplastic pollution is a problem that is made worse by complicated social and economic problems and changing environmental forces.

Conclusion:

Microplastic contamination is a growing global environmental problem that affects many different aquatic environments and has many different effects on creatures, ecosystems, and human health. Microplastics come from two main sources: primary and secondary. They are also found in many different types of pollution, such as wastewater effluent, worn-out fishing gear, and urban runoff. This is why they are so common in both surface waters and deep sediments. From an ecological standpoint, microplastics cause physical and physiological damage at all levels of the food chain, make pollutants build up more quickly, and throw food webs off balance. The primary harm to human health comes from eating seafood that has been polluted. Analytical methods have improved their ability to find things, but they still have problems with standardization and throughput. This shows that we need to keep improving our methods. India's situation shows how big the problem is and how new ways to fix it are coming up, such as bans on plastic, better waste management, and new bioplastics. It also shows how hard it is to enforce and build the right infrastructure. Future research goals focus on evaluating long-term effects, understanding nanoplastic behavior, and achieving worldwide standardization of analytical techniques to facilitate comprehensive

risk assessment and policy formulation. To reduce microplastic pollution, we need to work together to improve treatment technology, create better regulations, and raise public awareness. This is an important way to protect the health of aquatic ecosystems and people around the world.

Acknowledgment

I would like to express my sincere gratitude to all those who have contributed to the successful completion of this review titled "Microplastic Pollution in Aquatic Ecosystems: A Comprehensive Review of Environmental Impacts and Potential Solutions."

First and foremost, I extend my heartfelt thanks to my project guide for their invaluable guidance, continuous support, and insightful suggestions throughout the preparation of this review. Their expertise has greatly enhanced the quality of this work.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030105

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465270

DOI Link:
https://doi.org/10.5281/zenodo.19465270

Volume: 3

Issue: 1(I)

Pp. 30-33

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 10 Jan. 2026

Revised: 20 Jan. 2026

Accepted: 03 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Balusani, R., & Bandi, J. (2026). Validated Indirect Spectrophotometric Determination of Selected Drugs via Cerium (IV)–Methylene Blue Redox Reaction. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 30–33. https://doi.org/10.5281/zenodo.19465270

Validated Indirect Spectrophotometric Determination of Selected Drugs via Cerium (IV)-Methylene Blue Redox Reaction

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Abstract

The assay of Imatinib Mesylate (ITM) and Oseltamivir Phosphate (OSP) in bulk and tablet dosage form has been created in a simple, sensitive, accurate and cost-effective spectrophotometric process. This is done by oxidizing the drugs with a known excess of known excess of Ceric Ammonium Sulphate (Ce (IV)) in sulphuric acid medium. The number of unreacted Ce (IV) is estimated with Methylene Blue dye at the wavelengths of 664 nm. The process is in accordance with the Beer law at 321 mcg mL -1 (ITM) and 3.524.5 mcg mL -1 (OSP). Standard parameters of validation like LOD, LOQ, accuracy, precision, robustness and ruggedness were verified in line with ICH requirements. The process exhibited high recovery (>99 100) and low percentage RSD (< 2) that suggest that the method is applicable in the field of pharmaceutical routine analysis. Subjects: Spectrophotometry, Cerium (IV), Methylene Blue, Imatinib, Oseltamivir, Validation.

Keywords: *Indirect spectrophotometry, Cerium (IV) oxidation, Methylene blue reduction, Redox reaction, pharmaceutical analysis, Drug determination, Analytical method validation, UV-Visible spectrophotometry, Oxidative coupling reaction, Quantitative analysis*

Introduction

Imatinib mesylate (ITM) is an anticancer agent that is widely used in the management of chronic myeloid leukemia (CML) and gastrointestinal stromal tumor (GIT) [1]. It inhibits the tyrosine kinases, such as Bcr-Abl and was approved by US FDA in CML 2. It is 4-[(4-methyl-1-piperazinyl) methyl]-N-[4-methyl-3-[[4-(3-pyridinyl)-2-pyrimidinyl] amino] phenyl] benzamide monomethylan sulfonate 3. A number of methods of analysis have been used to estimate its estimation including UV spectrophotometry 4, HPLC 5, charge transfer complex 6, and RP-HPLC 7.

Oseltamivir Phosphate One of the neuraminidase inhibitors is Oseltamivir Phosphate which is an ester prodrug 8. It prevents influenza virus A and B viruses by blocking neuraminidase and is useful in preventing viral replication of the influenza virus 3. It is a 4-acetylamino-5-amino-3- (1-ethylpropoxy)-1-cyclohexene-1-carboxyllic acid ethyl ester. The UV spectrophotometry, 1 HPLC, RP-HPLC, HPTLC, colorimetric and chromatographic, 14 are some of the reported methods of analysis, and numerous others are available, but no easy oxidative spectrophotometric method has been reported. This experiment proposes that determination of these drugs could be done using KMnO 4Methylene Blue dye system as the analyzer

Principle Of the Method

Cerium (IV) sulphate is a strong oxidizing agent. The drugs reacted with a known excess of Ce (IV) in acid medium. The remaining Ce (IV) oxidizes Methylene Blue dye and the remaining dye absorbance is determined at 664 nm. The concentration of drugs is directly related to the absorbance.

Experimental

Instrumentation: Instrumentation: UV-Visible spectrophotometers (ELICO 210, Thermo Nicolet 1000, ELICO 159) with 10 mm quartz cells were applied.

Reagents: Cerium (IV) sulphate (4.0 10 -3 M), Methylene Blue (200 2g ml -1), Sulphuric acid (2 N). The appropriate dilution of standard drug solutions (200 µg mL -1) was made.

Procedure

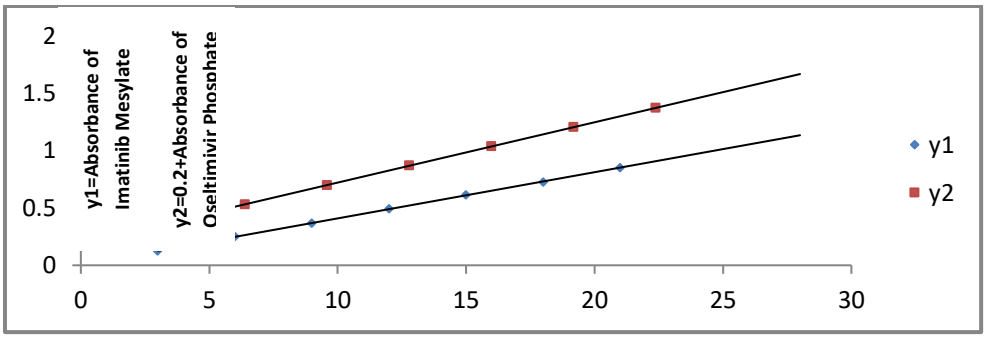
Aliquots of drug solution were mixed with 1 mL Ce (IV) and 1 mL 2 N H2 SO 4. After 15 minutes, 1 mL Methylene Blue was put there and diluted to 10 mL. The absorbance at 664 nm was taken as against reagent blank.

Assay Of Pure Drug Sample

Assays of standard solutions within the law limits established by Beer were done and recovery studies were done to determine accuracy and precision.

The data (Table 2) revealed a high percentage of recovery of less than 2% percent RSD indicating a high level of reliability of the methods.

Fig.3. Calibration curves of drugs ITM and OSP.



Concentration of drugs (µg mL^{-1})

Procedure For Assay of Pure Drug Standard solutions within Beer's law limits were analyzed and recovery studies were performed to evaluate accuracy and precision. The results (Table 2) showed excellent recovery with %RSD < 2%, confirming method reliability.

Procedure For Analysis of Tablets

Imatinib Mesylate

The stock solution was prepared by powdering tablets (Veenat 100 mg) and 10 mg of the powdered sample was dissolved in the double-distilled water and filtered and diluted to 100 mL. Analysis Analysis was carried out by the use of proper dilutions.

Oseltamivir Phosphate

To get the stock solution, the capsules (Tamiflu 75 mg) were broken, and the powder dissolved in two-distilled water in 10 mg then filtered and diluted to 100 mL. Further dilution was made where needed.

Method Of Validation

The procedures were evaluated in terms of linearity, accuracy, precision, LOD, LOQ, selectivity and ruggedness. Precision (n=6) and accuracy (percent recovery, percentRSD, < 2) were used to obtain method reliability (Table 2). LOD and LOQ were calculated as:

LOD = 3.3 S_a / S

LOQ = 10 S_a / S

S is the standard deviation of the intercept and S is the slope. The experiments of selectivity and ruggedness did not show any serious interference or variation. Absorbance is affected by 8 Factors.

Factors Affecting Absorbance

The Sulphuric acid was found to be the most suitable medium. The 1 mL of 2 N H 2 SO 4 was used to produce the maximum absorbance. The most appropriate reaction time was established to be 15 minutes and the reaction completion and constant absorbance were accomplished.

Analysis Of Pharmaceuticals

The formulations in tablet form showed a high recover (99100), low percentage-ratio-standard-deviation (2) meaning they can be used in the routine analysis.

Results And Discussion

This principle resembles the oxidation of drugs by excess Ce (IV) in an acidic environment, and the determination of any remaining oxidant with Methylene Blue at 664 nm. Increased concentration of drugs reduces effect of bleaching of the dye resulting in subsequent increase in absorbance. Under the use of 1 mL of 2 N H 2 SO 4, the best conditions were obtained.

Analytical Data

There was a strong relationship between absorbance and the concentration of the relationship. The great sensitivity and reliability of the method were verified by LOD, LOQ and regression parameters. [Table 1].

Table 1: Analytical and Regression parameters of Spectrophotometric Method

Name of drug Property	ITM	OSP
λ_{max}, nm	664	664
Beer's law limits (µg mL^{-1})	3.0-21.0	3.5-24.5
Molar absorptivity	2.07x10^4	1.39x10^4
Sandell's sensitivity (µg cm^{-2})	0.0259	0.0305
Variance $(S_a)^2$	0.00004	0.000002

Limit of detection µg mL^{-1}	0.1808	0.1713
imit of quantification µg mL^{-1}	0.5481	0.5192
Regression equation, Y**		
Intercept, (a)	0.0073	0.0029
Slope, (b)	0.0374	0.0312
Correlation coefficient, (r)	0.9995	0.9998
Standard deviation of intercept (S_a)	0.0020	0.0016
Standard deviation of slope (S_b)	0.0015	0.0021

Limit of determination is the weight in 0.0010 g/mL of solution that gives the absorbance of A = 0.001 measured in a cuvette of cross-sectional area of 1 cm2 with a path length of 1 cm. Y = a +bX, where Y is the absorbance, and X is the concentration of drugs in 0.0010 g/mL solution.

Accuracy And Precision

The correctness and accuracy was examined by measuring pure drugs with six chemical concentration levels in the working limits. According to Table 2, the method is nearly accurate and precise as the value of the relative error (%) and the RSD (%) of the data are high.

Table 2: Determination of accuracy and precision of the methods on pure drug Samples.

Drug	Taken (µg/ml)	Found (µg/ml)	error (%)	Recovery (%)	RSD (%)	Proposed method Mean ± SD
ITM	3.0 6.0 9.0	2.99 6.01 8.98	0.33 0.17 0.22	99.66 100.17 99.78	0.0851	99.75 ±0.0849
OSP	3.5 7.0 10.5	3.49 7.01 10.51	0.28 0.14 0.09	99.71 100.14 100.09	0.2349	99.98 ±0.2348

Robustness And Ruggedness: In the robustness assessment among the experiments, minor adjustments were performed on the reaction time and acid volume. Ruggedness was determined using different spectrophotometers and various analysts. No drastic changes were involved so that reliability of method was guaranteed.

Application To Formulations: The usefulness of the procedure was applied to the analysis of tablets without the interference of excipients. Results were in line with the methods and tests (t-test and F-test) reported that showed no significant difference at 95% level of confidence. Recovery levels (50-150 percent levels) provided satisfactory recoveries and confirmed accuracy and validity.

Table 3 Results of assay of tablets by the proposed methods and statistical evaluation and recovery experiments by the standard addition method.

Tablets	Drug in tablet µg mL^{-1}	Drug added µg mL^{-1}	Total found µg mL^{-1}	Error (%)	Recovery (%)	RSD (%)	Reference method Mean± SD	Proposed method Mean± SD
Veenat (ITM)	0.50 0.50 0.50 3.0 6.0 9.0	3.0 6.0 9.0 0.0 0.0 0.0	3.51 6.48 9.52 3.00 5.99 9.01	0.28 0.31 0.21 0.00 0.16 0.11	100.28 99.69 100.21 100.00 99.83 100.11	0.2255	100.5 ±0.55 (n=3)	100.021±0.2256
Oseltimivir Phosphate (OSP)	0.50 0.50 0.50 3.5 7.0 10.5	3.5 7.0 10.5 0.0 0.0 0.0	3.99 7.52 11.0 3.49 7.01 10.52	0.25 0.27 0.00 0.28 0.14 0.19	99.75 100.27 100.00 99.71 100.14 100.19	0.2164	100.30 ±0.1 (n=6)	100.01 ±0.2163

Table 4: F-test and t-test values

	Veenat (ITM)	Oseltamivir Phosphate (OSP)
F-test*	0.302 (4.7571)	0.01 (4.2839)
t-test**	0.981 (3.182)	1.195 (2.447)

t- test and F-test values from literature.

Conclusion

The paper describes an easy, delicate, accurate and fast spectrophotometric method of the identification of the selected drugs including the use of Cerium (IV) sulphate as the oxidizer. Excipients did not interfere with the technique and can be applied to pure drugs and pharmaceutical formulations. It is also an acceptable alternative to the existing methods of analysis.

Acknowledgement

The authors thank Prof. M. Sayaji Rao (Retd.), Department of Chemistry, University College of Science, Osmania University, for guidance.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| *Volume-3 Issue-1(I)* | *February-2026* | *ISSN: 3066-0637* | *Website:* https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030106

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465349

DOI Link:
https://doi.org/10.5281/zenodo.19465349

Volume: 3

Issue: 1(I)

Pp. 34-36

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 10 Jan. 2026

Revised: 20 Jan. 2026

Accepted: 03 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Sowbhagyam, D. V., & Kumar Goud, P. V. (2026). Green Chemistry as A Foundation for Sustainable Development: Innovations, Practices, And Global Implications. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 34–36.
https://doi.org/10.5281/zenodo.19465349

Green Chemistry as A Foundation for Sustainable Development: Innovations, Practices, And Global Implications

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Abstract

A sustainable society depends on chemical products and processes that are designed from the earliest molecular stage to support human health and environmental well-being [1, 2]. Evaluating whether a chemical is renewable, hazardous, or persistent requires attention to its inherent molecular characteristics during the design process [2, 6]. By integrating the principles of green chemistry and green engineering into raw materials, technologies, and manufacturing methods, it becomes possible to create chemical systems that meet performance expectations while also protecting the environment [1, 7]. Achieving this transition calls for combining long-standing scientific knowledge with modern approaches in systems thinking and design [8]. Beginning at the molecular level, these changes can ultimately contribute to global improvements in sustainability [9].

Keywords: *Green Chemistry, Sustainability, Materials Science, Agrochemical*

Introduction

Green chemistry, often called sustainable chemistry, focuses on creating chemical products and processes that reduce or eliminate the use and formation of harmful substances [2, 7]. The primary objective of this field is to lessen the negative effects of chemical activities on the environment and human health [1, 8]. The twelve principles of green chemistry, developed to guide the creation of safer and more sustainable chemical technologies, emphasize concepts such as preventing waste, reducing toxicity, and improving energy efficiency [2, 6]. These principles encourage the development of chemical processes that are sustainable from environmental, economic, and social perspectives [1, 7].

A critical component of green chemistry is the consideration of the entire life cycle of a chemical product [3, 9]. Rather than focusing only on synthesis, green chemistry evaluates the impacts of use, disposal, and long-term environmental consequences. By using this holistic approach, scientists aim to create chemical solutions that function effectively while minimizing harm over time [2, 4]. Industries ranging from pharmaceuticals to materials science have increasingly adopted green chemistry ideas to reduce their environmental footprint [4, 9]. Innovations in renewable feedstocks, green solvents, and biodegradable products reflect the growing importance of sustainability in industrial practices [5, 7]. As environmental pressures such as climate change and resource depletion intensify, green chemistry plays an essential role in building a more responsible and resilient chemical industry [8, 9].

Principles of Green Chemistry

The principles of green chemistry provide a framework for designing chemical processes that reduce harm and promote sustainability [2, 7]. Waste prevention encourages avoiding unwanted by-products from the beginning. Atom economy ensures that as many atoms as possible from starting materials remain in the final product [2, 4]. Designing less hazardous synthetic methods promotes the use of substances that pose fewer risks to humans and the environment [2, 6]. Creating safer chemicals ensures that products function effectively without causing unnecessary harm. Choosing safer solvents and auxiliary substances reduces exposure to toxic materials [5]. Energy efficiency encourages performing reactions under mild conditions to minimize energy use. Using renewable feedstocks supports the shift away from limited fossil resources [2, 6]. Reducing unnecessary chemical modifications lowers waste and resource consumption. Catalysis increases reaction efficiency and decreases the need for harsh conditions [2, 9]. Designing for degradation ensures that products break down safely after their useful life. Real-time monitoring helps prevent the formation of hazardous substances during production. Inherently safer design focuses on reducing the potential for accidents such as fires and explosions [2, 10]. Together, these principles guide the development of safer and more environmentally responsible chemical technologies.

Applications of Green Chemistry

Green chemistry plays an important role across many industries by reducing environmental impact and improving safety [1, 4]. In pharmaceuticals, environmentally friendly synthesis routes, reduced reliance on toxic solvents, and improved waste management contribute to cleaner production methods [4, 9]. Agrochemical development has benefited from safer pesticide design, renewable feedstocks, and farming practices that minimize chemical inputs [6, 8]. Materials science applies green chemistry through biodegradable polymers, energy-efficient synthesis, and recyclable material design [5, 7]. Energy production incorporates green chemistry principles in renewable energy technologies, improved catalysts, and sustainable fuel production [1, 9]. Water treatment increasingly uses biodegradable agents, energy-efficient purification systems, and biologically based treatment processes [6, 7]. The textile industry applies sustainable dyeing and finishing methods, while the food industry uses green processing techniques, eco-friendly packaging, and natural additives to reduce environmental impact [1, 7]. Green chemistry also guides the creation of safer cleaning products and supports waste management strategies that emphasize recycling and reduced pollution [9, 10]. Education and policy development continue to encourage wider adoption of sustainable chemical practices [8].

Pharmaceutical Applications

Green chemistry supports safer, more efficient, and less resource-intensive drug production methods [4, 9]. Greener solvents such as water or bio-derived liquids help reduce exposure to hazardous substances. Catalysis allows reactions to proceed more efficiently while minimizing energy consumption and chemical waste [2, 9]. Atom economy principles encourage synthetic routes that incorporate the maximum number of atoms into the final product [2, 4]. Environmentally friendly synthesis strategies rely on renewable feedstocks and biobased materials. Biocatalysis, which uses enzymes to drive chemical reactions, enhances selectivity while reducing the need for harsh conditions [4, 9]. Microwave and ultrasound-assisted synthesis shorten reaction times and lower energy use. Continuous flow chemistry improves control over reaction conditions and reduces waste generation [4]. Green analytical methods help monitor pharmaceutical processes without hazardous reagents. Recycling strategies and reduced waste production further improve sustainability. Biodegradable packaging materials contribute to environmental protection, while life cycle assessments help evaluate the full environmental impact [1, 9].

Agrochemical Applications

Applying green chemistry in agriculture supports the development of safer and more sustainable agrochemicals [6, 8]. Efficient synthesis pathways that maximize atom usage reduce waste. Choosing water-based or low-toxicity solvents lowers environmental impacts [5]. Catalytic processes make production more efficient and reduce energy inputs. Renewable raw materials lessen dependence on nonrenewable resources. Designing chemicals that pose fewer risks to humans, beneficial insects, and ecosystems improves agricultural safety [6, 8]. Precision application techniques ensure chemicals are used only where needed, reducing environmental load. Biodegradable formulations prevent long-term soil and water contamination. Environmentally friendly analytical methods support monitoring and regulation, while integrated pest management combines biological and chemical approaches [6]. Innovative delivery systems improve efficiency and reduce overall chemical usage.

Materials Science

Green chemistry has transformed materials science by promoting solutions that reduce environmental impact and improve product safety [5, 7]. Biodegradable polymers provide alternatives to conventional plastics that persist in the environment. Renewable raw materials support sustainable manufacturing. Replacing hazardous solvents with safer options such as water protects workers and reduces air pollution [5]. Energy-efficient synthesis techniques, including microwave-assisted methods, decrease resource consumption. Catalysis improves reaction efficiency and reduces unwanted by-products. Designing recyclable materials supports circular economy goals. Minimizing toxicity during materials production protects human health and the environment. Life cycle assessments offer a comprehensive view of a material's environmental impact [3, 7].

Energy Production

Green chemistry contributes to sustainable energy production by guiding the development of clean technologies and environmentally responsible materials [1, 9]. Solar energy research focuses on durable and nontoxic materials for photovoltaic systems. Wind energy technologies incorporate recyclable components and environmentally friendly lubricants and coatings. Bioenergy production benefits from green chemistry through the use of nonfood biomass sources and efficient conversion processes. In energy storage, green chemistry promotes safer battery materials and recyclable components [1, 9]. Sustainable hydrogen production relies on catalysts made from abundant and nontoxic elements. Carbon capture technologies use greener solvents and catalytic processes to reduce emissions, and converting captured carbon into valuable chemicals or fuels supports resource efficiency [2, 9].

Water Treatment

Water treatment increasingly benefits from green chemistry principles [6, 7]. Alternative treatment agents such as natural polymers and biodegradable coagulants replace traditional chemicals that pose environmental risks. Optimizing chemical usage reduces waste and contamination. Energy-efficient methods, including ultraviolet purification, membrane filtration, and electrochemical systems, lower overall resource consumption. Safer solvents minimize the release of harmful substances during treatment. Biological techniques such as phytoremediation and microbial filtration harness natural processes to remove contaminants efficiently.

Food Technology

Green chemistry enhances sustainability in food production [1, 7]. Organic fertilizers, biopesticides, and green farming techniques help reduce chemical burdens on the environment. Biodegradable packaging materials replace conventional plastics. Efficient processing technologies and innovative extraction methods reduce reliance on hazardous solvents. Renewable energy sources contribute to cleaner food manufacturing. Green ingredients from natural or renewable sources provide safer preservatives, antioxidants, and antimicrobials. Water-saving techniques reduce resource use. Biotechnology-based processes produce ingredients more efficiently and with fewer environmental impacts. Life cycle assessments guide improvements throughout the production chain, and educational initiatives support the training of food scientists in sustainable practices [9].

Conclusion

Progress in research and international environmental cooperation has supported the growth of sustainable chemical technologies [1, 2, 9]. Yet many industries still face challenges in evaluating the economic practicality of adopting green chemistry on a wide scale. Continued investment, improved education, and a stronger emphasis on the benefits of green chemistry are essential for advancing sustainable chemical manufacturing. By highlighting its positive effects on environmental protection, worker safety, pharmaceutical development, and public health, green chemistry can continue to drive meaningful improvements in industrial practices and long-term sustainability [1, 4, 8].

Acknowledgment

I would like to express my sincere gratitude to all those who have contributed to the successful completion of this study titled "Green Chemistry as a Foundation for Sustainable Development: Innovations, Practices, and Global Implications."

First and foremost, I extend my heartfelt thanks to my project guide for their invaluable guidance, constant encouragement, and insightful suggestions throughout the course of this work. Their expertise has greatly contributed to the development of this study.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030107

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465401

DOI Link:
https://doi.org/10.5281/zenodo.19465401

Volume: 3

Issue: 1(I)

Pp. 37-41

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 10 Jan. 2026

Revised: 20 Jan. 2026

Accepted: 03 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
K. Naresh, V. Shekar, Narsimha, D. B., & M. Nagu. (2026). Applications of Superconductivity in Medicine, Power Systems, and Transportation: A Comprehensive Review. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 37–41.
https://doi.org/10.5281/zenodo.19465401

Applications of Superconductivity in Medicine, Power Systems, and Transportation: A Comprehensive Review

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Abstract

Superconductivity is a phenomenon of exactly zero electrical resistance and expulsion of magnetic flux fields occurring in certain materials when cooled below a characteristic critical temperature. Superconductivity is a quantum mechanical phenomenon and it is characterized by the Meissner effect, the complete ejection of magnetic field lines from the interior of the superconductor as it transitions into the superconducting state. Superconductors offer major advances in efficiency and performance in electric power generation, transmission and storage; wireless communications; computing; transportation and scientific instruments that are cost effective and environmentally friendly. Superconducting materials have a significant role in advancing industrial and scientific applications with major benefits in various sectors including energy, environment, and healthcare. Superconductors are used to make devices known as a superconducting quantum interference device (SQUIDs), which are used in scanning SQUID microscopes and magneto encephalography. Superconducting magnets are some of the most powerful electromagnets known. They are used in MRI/NMR machines, mass spectrometers. Levitating trains have been built that use powerful electromagnets made from superconductors. More recently, superconductors have been used to make digital circuits based on rapid single flux quantum technology and RF and microwave filters for mobile phone base stations.

Keywords: *Superconductivity, Zero Electrical Resistance, Meissner Effect, High-Temperature Superconductors (HTS), Low-Temperature Superconductors (LTS), Magnetic Resonance Imaging (MRI), Particle Accelerators, Superconducting Magnets, Power Transmission, Superconducting Cables*

Introduction

Superconductivity is a phenomenon of exactly zero electrical resistance and expulsion of magnetic flux fields occurring in certain materials when cooled below a characteristic critical temperature. On April 8, 1911, Dutch physicist Heike Kamerlingh Onnes made the discovery at Leiden. Superconductivity is a quantum mechanical phenomenon, just like ferromagnetism and atomic spectral lines. Three key characteristics of superconductivity are macroscopic quantum processes, a completely diamagnetic Meissner effect, and zero DC resistance. In the presence of a static magnetic field, superconductors create a spontaneous and nearly full diamagnetic response, which is the second characteristic. The material will create currents to keep the magnetic field out of its interior while it transitions into the superconducting state. The Meissner effect is a phenomenon that sets superconductors apart from perfect conductors, which wouldn't exhibit a spontaneous Meissner effect. Lastly, the quantum mechanical character of the superconducting correlated electron state gives rise to macroscopic quantum effects.

The electromagnetic properties of superconductors are intriguing and distinct. The electromagnetic response of a superconductor can be understood in terms of the two fluid models, a simplistic but reasonably useful model. A super-fluid of Cooper-paired electrons and a second fluid of "normal," or non-superconducting, electrons coexist to form the superconductor. These two fluids respond differently to electromagnetic fields. The diamagnetic Meissner state is established and maintained below the critical temperature Tc by the super fluid, which responds to external fields in a purely reactive (inductive) manner. The majority of the dissipative characteristics of the superconducting state are caused by the normal fluid's absorption of photons, which functions like a collection of regular electrons.

Superconductivity is present in numerous compounds and throughout the periodic table. Because their transition temperatures ranged from a few mK to roughly 25 K, traditional (pre-1986) superconductors are sometimes referred to as "low-Tc" superconductors. The "high-Tc" superconductors have transition temperatures of up to 150 K and are mostly based on copper oxide. More lately, some intriguing new superconductors, such as MgB2 and iron-pnictide superconductors, have been found in the intermediate temperature range of 5 K to 50 K.

Nb (Tc = 9.2 K) and certain alloys (e.g., Nb-Ti) that are utilized to make superconducting magnets for particle accelerators and magnetic resonance imaging are technologically significant superconductors.

Applications in Medicine:

SQUID Magnetometer

The SQUID magnetometer is one of the main proponents of super conduction. Superconducting Quantum Interference Device is referred to as SQUID. This measurement tool is among the most sensitive magnetic measurement tools available since it can detect magnetic fields in the femto-tesla range. Even though the human body produces quite tiny magnetic fields, measuring these fields has significant diagnostic significance. The SQUID magnetometer is the primary instrument used to measure these fields. A Josephson junction is created when two superconductors are connected by a weak link. There are several ways to create such a weak connection. One or two of these junctions in a superconducting loop make up a SQUID magnetometer. For the detection of bio magnetic signals, the DC-SQUID with two Josephson junctions is nearly always utilized. The SQUID loop should be as tiny as feasible to maintain low inductance; a pickup loop is required if the sensor loop is small but highly sensitive. While some high temperature superconductors include a directly connected pickup loop, this loop often links inductively with the SQUID loop. Some readout electronics are also required in addition to the sensor.

Magnetoencephalography

Using extremely sensitive magnetometers, magnetoencephalography (MEG) is a functional neuroimaging method that maps brain activity by capturing magnetic fields generated by electrical currents that naturally occur in the brain. The majority of bio-magnetic signals originate from intracellular current flow brought on by cerebral or muscle stimulation. An extracellular current flow via the volume conductor completes the circuit; these cells serve as the current source. EEG methods can be used to measure the quantifiable electric fields produced by this current flow. Additionally, it produces a measurable but extremely faint magnetic field. Measuring the magnetic field has the benefit of measuring the currents that are vertical to the surface of the body. These currents are mostly caused by intracellular current flow, which is less distorted than volume current and enables MEG to achieve far better resolutions than EEG. Because the two readings are complementary, it can also be utilized in conjunction with EEG techniques.

Typically, MEG systems are made up of a dewar that encircles the entire head and contains a variety of low temperature SQUID sensors. Typically, the array is made up of 37 to 255 SQUID sensors, either in a magnetometer or gradiometer format, with a few sensors set aside for noise cancellation. Two pickup coils are positioned on a baseline in a gradiometer configuration so that the magnetic fields passing through them cancel out and only the difference is magnified. A single pickup coil with a SQUID sensor makes up the magnetometer. MEG measurements are always conducted in a magnetically protected chamber due of the small signal sizes. Numerous clinical and research applications make use of MEG. It is employed to study other even more intricate brain activities as well as temporal elements of signal processing in the brain. MEG offers numerous more special study uses when combined with PET, MRI, fMRI, and EEG.

Magnetocardiography

Magnetocardiography (MCG) is a technique to measure the magnetic fields produced by electrical activity in the heart using extremely sensitive devices such as the superconducting quantum interference device (SQUID). If a multichannel device is used to measure the magnetic field, a map of the magnetic field across the chest is produced. From this map, the source of the activity can be found using mathematical algorithms that account for the torso's conductivity structure.

An array of SQUID sensors, which typically cover the entire chest region—sometimes even the front and back—is another component of the basic MCG device. There are anywhere between seven and sixty-four sensors. Every model—aside from a few experimental models—operates in a magnetic protected space. MCG is used in patient screening because it requires significantly less setup time than ECG readings. Together with the catheter approach, it has also been utilized to map cardiac arrhythmias. The MCG is utilized to map the catheter position as a more accurate measurement of the area to be ablated once the arrhythmia has been generally localized. MCG is used to predict myocardial ischemia and has been demonstrated to predict malignant cardiac arrhythmias with significantly higher accuracy than ECG. Fetal magnetocardiography is a major application that is emerging in the field of MCG. MCG has significant clinical value for the analysis of fetal heartbeat in high-risk pregnancies since it is not subject to the considerable distortion that fetal ECG is prone to because of an isolating layer called the vernix caseosa.

Magnetic Resonance Imaging (MRI)

MRI (Magnetic Resonance Imaging) scanning is a medical investigation that uses an exceptionally strong magnet and radio frequency waves to generate image of your body. One of the most advanced diagnostic methods available to assist a referring physician in determining the root cause of your specific health problem is an MRI scan.

MRI scanners rely on superconductivity to provide physicians with a previously unattainable glimpse of deep within the human body.

The magnet is the largest and most crucial part of an MRI machine. The patient enters a horizontal tube that passes past the magnet from front to back. The bore is the name for this tube. However, this isn't just any magnet—we're working with a very powerful device that can generate a sizable, steady magnetic field. A magnetic field of 0.5 to 2 Tesla (5,000 to 20,000 gauss) is produced by the magnets now used in MRI equipment. You can see how strong these magnets are when you consider that the Earth's magnetic field is 0.5 gauss.

A superconducting magnet, which is made up of several wire coils or windings through which an electrical current is transmitted, is used in the majority of MRI machines. Compared to resistive electromagnets, these superconducting magnets have several advantages. Compared to standard ferromagnetic-core electromagnets, which can only produce fields of about 2 T, they can produce magnetic fields that are up to ten times stronger. Measurements are less noisy since the field is typically more steady. Superconductivity, or lowering the resistance in the wires to nearly zero, provides the energy needed to maintain such a strong magnetic field in MRI. The cables are continuously submerged in liquid helium to accomplish this. A vacuum acts as insulation against this cold. Superconductivity keeps the system cost-effective, and the powerful magnetic field enables the best picture quality despite the high cost of superconductive magnets.

Applications in Power System:

Superconducting Generators

Superconducting elements are the most important part of electromechanical systems because of their functioning and these systems form the superconducting electric machines. Lack of DC resistance in super conductors contributes much to its greater efficiency. In a super conducting machine very high magnetic field is produced otherwise impossible in a conventional machine and is the main characteristic of super conductors. High magnetic field results in lesser motor volume and ultimately more power density. Compared to ordinary generators, superconducting generators have three possible advantages. They provide improved system stability against frequency fluctuations brought on by grid transients. They can function at higher magnetic fields (5 to 6 tesla), which allows for a 50% reduction in size. This could lead to a large reduction in capital expenses. Lastly, a 0.5% gain in efficiency would result in a roughly 50% decrease in losses. Over the generator's lifespan, fuel savings from even this tiny efficiency boost might cover its initial expenditures.

Superconducting generators today use the same operating principle as older electric generators, such as synchronous permanent magnet generators or motors and induction machines. The superconducting generator's windings are the only distinction between the two. Compared to traditional generators, these windings can sustain a stronger magnetic field. Using this coil in other rotating devices will increase their efficiency and make them more environmentally friendly and compact. The superconducting generators feature a damper to protect the coil from high frequency magnetic fields and a coil cover to maintain the coil under centrifugal force. Along with a rotary seal, which is a rotating room that supplies the cryogenic coolant, there is a cooling chamber to maintain an extremely low temperature. The core consists of a copper stator coil and a non-magnetic stator core. Through the slip ring, the super conducting coil, which is composed of superconducting material, receives the current. Additionally, there are three insulations: the torque tube, which serves as the insulating structure, the vacuum jacket, which creates the vacuum insulation layer, and the shield, which guards against the discharge of magnetic field into the surrounding area.

Superconducting Magnetic Energy Storage (SMES)

Superconducting Magnetic Energy Storage (SMES) systems store energy in the magnetic field created by the flow of direct current in a superconducting coil which has been cryogenically cooled to a temperature below its superconducting critical temperature. In order to discharge the SMES and recharge it, power conditioning systems must transform the DC power in the magnet into AC for the grid. SMES could be used in electric utilities in a number of ways. Large units (capacity greater than 1 GW-hr) could be utilized for load levelling and diurnal storage. Numerous operational advantages, such as spinning reserve, autonomous generation management, black start capability, and enhanced system stability, may be offered by smaller units. Because SMES can supply massive amounts of pulsed power to weapon systems like ground-based lasers for ballistic missile defence, it is also of interest to the military.

The creation of a 20 MW-hr/400 MW engineering test model (ETM), which might start testing by 1993, is now being supported by the Initiative Organization (SDIO). Utilities are contributing a small portion of the funding through the Electric Power Research Institute because the military and utility designs are similar except for the power conditioning system (weapons must receive large amounts of power quickly and may drain the SMES in a very short time; utilities must have a constant reliable supply from which smaller amounts of power are withdrawn on a daily basis.

Utilities have experimented with a number of energy storage techniques, including as charging batteries and capacitors, compressing air, and pumping water uphill to a reservoir. Compared to other forms of energy storage systems, SMES has a number of advantages. It can transition between charging and discharging modes in a matter of milliseconds and offers a better efficiency than any other storage technology for load levelling—roughly 90–93 percent, as opposed to 70–75 percent for pumped hydro. Because of its rapid reaction time, it can help keep the utility system stable in the face of brief disruptions.

Power Transmission Lines

Superconducting Power Transmission Cables transmit 5 to 10 times the electrical current of traditional copper or aluminum cables with significantly improved efficiency. Superconducting power cable systems consist of the cable, which is comprised of 100's of strands of superconducting wire wrapped around a copper core, and the cryogenic cooling system to maintain proper operating conditions. Direct current (DC) or alternating current (AC) could be carried via superconducting transmission lines. Large power blocks are transported from one location to another via DC cables. High currents could be carried by a superconducting DC wire without any resistive losses. However, a superconducting line would need to be incredibly long (possibly several hundred miles) in order to be economically competitive with less expensive overhead lines because the conversion to AC at either end dominates the cost of DC lines.

Superconducting power cables serve as a link between the distribution and transmission of electric energy. Distribution voltages range from 5 kV to 46 kV, while transmission voltages range from 60 kV to 765 kV. This medium voltage feeds to load spots in crowded cities for superconducting cables. The grid is frequently overloaded with outdated infrastructure in these high demand areas. When building additional transmission to distribution substations with significant transformer assets is either not practical or cost-effective, HTS technology brings a significant quantity of power to new locations. Superconducting power cables are especially well-suited for high load locations, including the crowded urban business districts of big cities, where building and easement purchases for conventional low-capacity lines can be prohibitively expensive.

Applications in Transportation:

Applications of superconductivity in transportation include: magnets for levitation, propulsion, and guidance of high-speed ground vehicles; motors and generators for use in ships, aircraft, locomotives, and other ground vehicles; energy storage and propulsion systems for cars; and magnets for ship propulsion.

Maglev Systems

Magnetic levitation, or Maglev, is a mode of transportation that moves vehicles without coming into touch with the earth. Maglev vehicles use magnets to generate both lift and propulsion as they move along a guideway, greatly decreasing friction and enabling extremely high speeds. Maglev technology doesn't have any moving parts by itself. Compared to wheeled mass transit systems, maglev trains travel more silently and smoothly. As with other high-speed transportation, the majority of the power required for levitation is usually used to counteract drag. The train speed record is held by maglev trains.

For maglev vehicles, attractive force and repulsive force are the two main levitation ideas. Non-superconducting electromagnets installed on the vehicle that are drawn to the underside of steel rails are used in attractive maglev. The suspension gap between the automobile and the rails is less than half an inch, which puts stringent requirements on track alignment and is one drawback of this design. In repulsive-force maglev, also known as "electrodynamics," cars are levitated by superconducting magnets that create repulsive currents in a guideway made of coils or sheets of aluminium. Six to ten inches above the guideway, vehicles are levitated.

Japanese scientists used this technology of Electrodynamics Suspension (EDS) to levitate a train. This relies on electromagnetic induction, which causes a current to be induced when a magnet moves next to a conductor, altering the magnetic field inside the conductor. Lenz's Law states that the magnetic field created by the induced current tends to oppose the change that initiated the induction. The electromagnetic induction principle is used in the EDS approach. The train follows a guideway with a set of "8"-shaped coils on either side. The superconducting magnets on either side of the train will cause a current to flow through the coils as it passes quickly. The key is that the magnetic flux change in the lower half of the "8"-shaped coils is greater than that in the upper half because the superconducting magnet passes below the centre of the coils, inducing a current that produces a magnetic force. Both sides of the "8"-shaped coils produce an upward component of magnetic force on the superconducting magnet, which causes the train to levitate. The lower half of the coils has the same magnetic pole as the superconducting magnet, while the upper half has the exact opposite. The train cannot be levitated when it is at rest because the "8"-shaped coils can only produce magnetism and create a current when the superconducting magnets are moving. As a result, the train slides on its wheels to begin. The wheels are concealed like those of an airplane taking flight when the magnetic force produced is strong enough to overcome the train's weight.

Due to their much-reduced weight and power requirements, superconductor magnets are crucial to these maglev trains. Low temperature superconductor (LTS) technology is currently used on maglev train lines in China, Germany, and Japan. Nonetheless, studies are currently being conducted on the use of HTS coils in maglev trains, which may lead to reduced cooling expenses and improved stability.

Conclusion

Given that prediction of the future is always uncertain, it can be safely stated that superconductivity will continue to supply science with a magnificent platform and incentive for new discoveries and theories in condensed matter physics. It is clear that we do not yet know all the ways that the Cooper pairing phenomenon or zero-resistance coherent states can arise in condensed matter or the detailed properties of these states. The recent material discoveries discussed here offer solid evidence that materials research will continue to create new materials that could either improve upon existing ones or disclose these new phases in an experimental sense. If the HTS narrative is any indicator, the more practical work of transforming these new materials into commercially viable forms, from which application advantages may be gained, may produce the greatest future effort of all.

It should also be evident that developments in areas other than superconducting materials themselves—such as production techniques, insulation, cryogenics, cryo-refrigeration, and cost-cutting measures—are beneficial and essential to the continued success of superconducting applications. A superconducting design will always be in competition with alternative solutions, which might be more dependable or economical, unless there is no other way to tackle a problem. Although the other characteristics mentioned above are equally important, superconducting materials may most easily contribute to the endeavor by raising the available system operating temperature.

Acknowledgement
All the Authors are thankful to the Principal and HOD, Department of Chemistry, Government Degree College for Women(A), Nalgonda, Telangana, India for granting permission to carry out the work.

Financial Support and Sponsorship
Nil.

Conflicts of Interest
The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| *Volume-3 Issue-1(I)* | *February-2026* | *ISSN: 3066-0637* | *Website:* https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030108

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465452

DOI Link:
https://doi.org/10.5281/zenodo.19465452

Volume: 3

Issue: 1(I)

Pp. 42-45

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 10 Jan. 2026

Revised: 20 Jan. 2026

Accepted: 03 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
J. Madhavi. (2026). Effect of Co-Mo nitride catalyst over carbonaceous support in the Oxidative dehydrogenation of Ethylbenzene. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 42–45.
https://doi.org/10.5281/zenodo.19465452

Effect of Co-Mo nitride catalyst over carbonaceous support in the Oxidative dehydrogenation of Ethylbenzene

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Abstract

The oxidative dehydrogenation of ethylbenzene was conducted on 10 and 20wt% Co_3Mo_3N supported over carbonaceous support such as activated carbon under atmospheric pressure, employing various gas flows, including N_2, CO_2, and a CO_2-N_2 mixture. The catalyst with 10 wt% Co_3Mo_3N on activated carbon exhibited superior activity compared to the 20 wt% catalyst at all gas flows. Notably, the better dehydrogenation activity in case of 10 wt% catalyst under CO_2-N_2gas flow due to the synergistic effects of ammonia synthesis and the reverse water–gas shift reaction. All catalysts were characterized using XRD, TPR, BET surface area.

Keywords: *Ethylbenzene, Styrene, Co_3Mo_3N catalyst, Activated carbon*

Introduction

Styrene (ST) is an essential chemical species used in the production of several polymers. It is industrially produced via the dehydrogenation of ethylbenzene (EB) with the help of an iron oxide catalyst at temperatures between 873K to 973 K. Nevertheless, the dehydrogenation process is subjected to thermodynamic limitations and necessitatesa substantial energy input because of the extensive utilization of superheated steam. As an alternative, oxidative dehydrogenation (ODH) of EB has been proposed. Most research and development efforts concerning EB dehydrogenation have focused on identifying suitable catalysts and optimizing the reaction conditions to enhance the yield and selectivity of styrene [1-4].

Acidic oxide catalysts are susceptible to coke formation during ethylbenzene dehydrogenation. It has been documented that this carbonized coke functions as an active phase for catalytic dehydrogenation [5-8]. The quinone-type groups present on the coke surface serve as active sites for the dehydrogenation of ethylbenzene reaction [6, 9, 10]. These results indicate that carbonaceous materials, including activated carbon and graphite, can be used as catalysts for dehydrogenation reactions. Studies have indicated that high activity and selectivity can be achieved at relatively low temperatures when activated carbon used as a catalyst [11, 12]. The textural properties and surface functional groups of activated carbons (ACs) are influenced by the precursor used, as well as strategy and preparation conditions [13]. Several research groups have investigated the development of activated carbons with specific characteristics that render them suitable for use as catalysts in oxidative dehydrogenation (ODH) reactions [14]. In the present study, Co_3Mo_3N with 10 and 20 wt% loading supported on activated carbon wasutilized for the dehydrogenation of ethylbenzene under various gas flows [15].

Experimental

1. Catalyst preparation

The Co-Mo nitride catalysts with 10 and 20wt% compositions were synthesized by impregnating the activated carbon with an aqueous solution of mixed salt precursors. These precursors contained specified amounts of Co $(NO_3)_2.6H_2O$, $(NH_4)_6Mo_7O_{24}.4H_2O$, and HMT (M/s, Sigma Aldrich). This impregnated material was subjected to aerial evaporation and followed by drying at 313 K for 6 h. The resulting material was calcined under the flow of N_2gas as documented in the literature [15].

2. Catalyst characterization

The X-ray diffraction patterns of the catalysts, the BET surface area, and the temperature-programmed reduction were recorded in accordance with the methodologies reported in the literature [15].

3. Catalyst activity

The catalytic activity was conductedutilizing a fixed-bed downflow quartz reactor operating under atmospheric pressure. Approximately 1 g of catalyst was placed within the reactor, situated between two plugs of quartz wool at the reactor's center, and subjected to pretreatment at 873 K for 30 min under the nitrogen flow of 30 ml min^{-1}. The reaction was conducted at the temperatures of 773, 823, and 873 K, under different gas flows. The gas environments employed included N_2, CO_2, and mixtures of CO_2 and N_2. Ethylbenzene was introduced via syringe pump (M/s. B. Braun, Germany) at a feed rate of 8.2 mmol h^{-1}.

The reaction products were collected periodically in an ice-cold trap and analyzed using a flame ionization detector (FID) equipped with a gas chromatograph, GC-17A (M/s. Shimadzu Instruments, Japan) [15].

Results And Discussion

1. X-ray diffraction patterns

The XRD patterns of fresh Co_3Mo_3N, AC, 10 wt. % Co_3Mo_3N/AC, and 20 wt. % Co_3Mo_3N/AC catalysts are depicted in Figure 1. The XRD pattern of the bulk Co_3Mo_3N sample exhibited signals at 2θ values of 35.5°, 40.2°, 42.7°, 46.7, and 72.80. However, in the XRD pattern of 10 wt% Co_3Mo_3N/AC, peaks corresponding to Co_3Mo_3N were not observed. This absence may be due to the crystalline size of Co_3Mo_3N being below the detection limit of XRD or its amorphous phase. This observation agrees with the existing literature, which indicates that low loadings of Co_3Mo_3N do not exhibit signals attributable to bulk Co_3Mo_3N. In contrast, a higher loading of 20 wt% displayed well-known reflections associated with the bimetallic nitride phase [15].

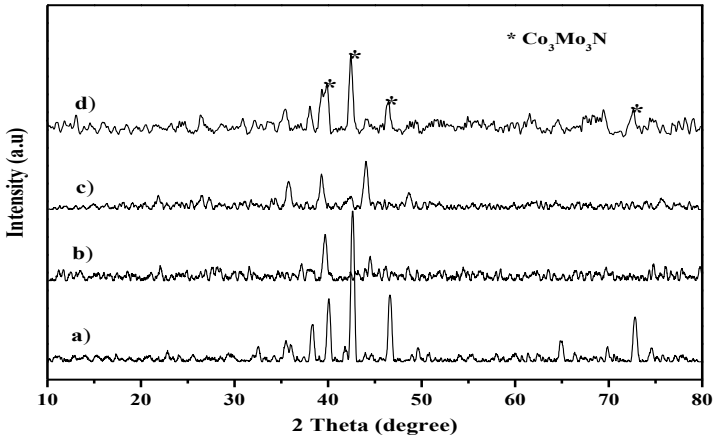


Figure-1: XRD patterns of **a)** Co_3Mo_3N, **b)** Activated carbon, **c)** 10wt% Co_3Mo_3N/AC and **d)** 20wt% Co_3Mo_3N/AC

2. BET surface area analysis

The BET surface areas of all the catalysts aregiven in Table 1. The surface area of the activated carbon was measured to be 905 $m^2\ g^{-1}$, which decreased by the deposition of the Co-Mo nitride. This decreasing trend in surface area persisted as the bimetallic nitride content increased from 10 to 20 wt. This phenomenon is expecteddue to the obstruction of the activated carbon pores by the Co-Mo nitride phase [15].

S. No	Catalysts	Surface area ($m^2\ gm^{-1}$)
1.	Activated carbon	905
2.	10wt% Co_3Mo_3N/AC	487.1
3.	20wt% Co_3Mo_3N/AC	412.5

Table 1: BET surface areas of activated carbon and Co-Mo nitride supported catalysts

3. TPR Analysis

The TPR profiles of the catalysts are illustrated in Figure 2. The TPR pattern of the Co_3Mo_3N catalyst, exhibited two T_{max} peaks. In the TPR pattern of the 10 wt% catalyst, Tmax was observed with negative intensity at elevated temperatures, which was attributed to methane formation due to carbon reduction. Conversely, in the TPR pattern of the 20 wt% catalyst, there was a shift in Tmax, due to the formation of larger particles (Figure 3c). The TPR pattern of the 20 wt% Co_3Mo_3N/AC catalyst also displayed a negative signal at higher temperatures, similar to the TPR pattern of the 10 wt% catalyst [15].

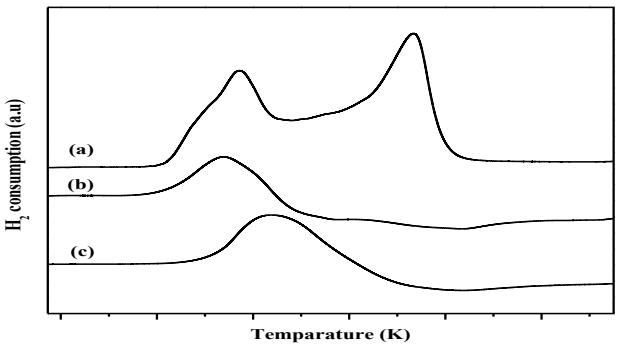


Figure- 2: TPR analysis of a) BMN, b) 10BMN/AC and c) 20BMN/AC catalysts

4. Activity studies

Studies on the dehydrogenation activity of ethylbenzene (EB) were conducted at 773, 823, and 873 K using 10wt%Co_3Mo_3N/AC and 20wt%Co_3Mo_3N/AC catalysts under a nitrogen flow (Figure 3). The 10wt% catalyst demonstrated an EB conversion rate of 46.6% at 873 K, which was higher than the 42% conversion rate observed with the 20wt% catalyst. This increased activity was attributed to the greater number of active sites present in the 10wt% Co_3Mo_3N/AC catalyst. Consequently, a time-on-stream study was performed using the 10wt% catalyst, and the results are depicted in Figure 3.

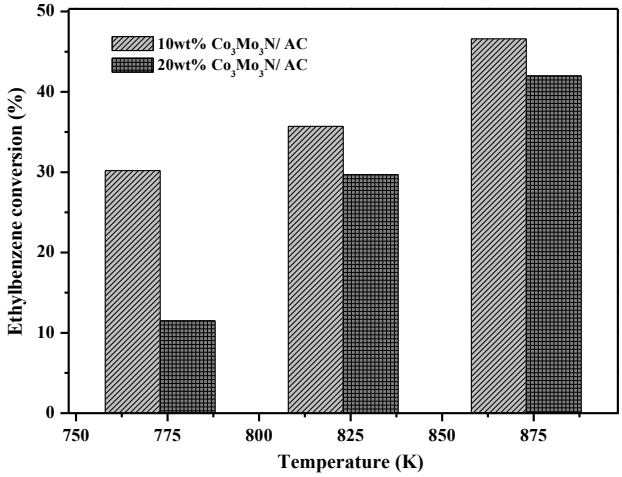


Figure-3: Investigation of temperature effects on the dehydrogenation of EB over 10 and 20wt% Co_3Mo_3N/AC in N_2 flow

Figure 4 illustrates the ethylbenzene (EB) dehydrogenation process over time with various co-feed gases. When nitrogen (N_2) was used as the co-feed, the conversion of EB was initially 53.6%, decreasing to 24% by the end of the sixth hour. This decline was attributed to the insufficient formation of ammonia (NH_3) in the N_2 flow, which was inadequate to neutralize the strong acidic sites of the catalyst, thereby reducing the EB conversion over time. In contrast, using carbon dioxide (CO_2) as the co-feed resulted in a higher EB conversion of 60.1% compared to 53.6% with N_2. This is because the equilibrium conversion of CO_2 in the reverse water-gas shift reaction (RWGSR) is significantly higher than that of NH_3 synthesis under comparable conditions. Consequently, the CO_2 co-feed was more effective in enhancing EB conversion than N_2. Moreover, the utilization of CO_2 and N_2 as co-feeds with EB further enhanced the EB conversion due to the interaction of two equilibrium- controlled reactions namely, RWGSR and NH_3 synthesis. Nevertheless, the amount of NH_3 generated t in situ was insufficient to neutralize the acidic sites present on the catalyst surface in presence of N_2, CO_2, and CO_2+N_2 flows, resulting in a significant decrease in the EB conversion. The reduction in conversion observed from the initial stage to the sixth hour was approximately 30% in all gas flows [15].

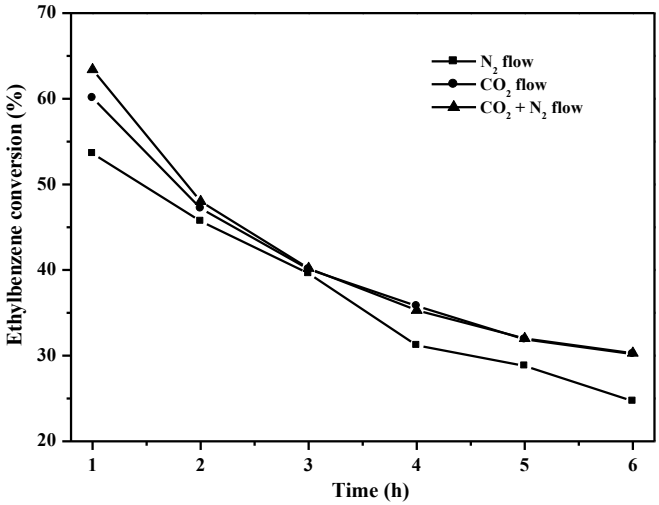


Figure -4: Time on stream studies on 10wt% Co_3Mo_3N/AC in different gas flows

Conclusion:

The 10 wt% Co_3Mo_3N catalyst supported on active carbon demonstrated superior activity compared to the 20 wt% catalyst, which was attributed to the effective dispersion of the nitride. Time-on-stream studies revealed a decline in the ethylbenzene conversion across all gas flows. Notably, the conversion of ethylbenzene was enhanced in the CO_2 + N_2 flow. The formation of ammonia was insufficient to neutralize the acidic sites, resulting in a decrease in the ethylbenzene conversion over time.

Acknowledgment

The authors express their sincere gratitude to their institution for providing the necessary facilities and a supportive research environment to carry out this work. We are deeply indebted to our research supervisor(s) for their constant guidance, valuable insights, and encouragement throughout the course of this study.

We extend our appreciation to the laboratory staff and technical personnel for their assistance in catalyst preparation, characterization, and experimental analysis. Their expertise and support were crucial to the successful completion of this research.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030109

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465497

DOI Link:
https://doi.org/10.5281/zenodo.19465497

Volume: 3

Issue: 1(I)

Pp. 46-48

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 10 Jan. 2026

Revised: 20 Jan. 2026

Accepted: 03 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Rao, D. V., & A Dayanand. (2026). Forever Chemicals (PFAS): Environmental Persistence and Chemical Remediation Strategies. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 46–48. https://doi.org/10.5281/zenodo.19465497

Forever Chemicals (PFAS): Environmental Persistence and Chemical Remediation Strategies

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Abstract

Per- and polyfluoroalkyl substances (PFAS) represent a chemically diverse class of anthropogenic fluorinated compounds whose environmental persistence is primarily governed by the extraordinary strength of the carbon–fluorine bond. Their widespread application in industrial processes and consumer products has resulted in global-scale contamination of aquatic systems, soils, atmospheric compartments, and biological tissues. Unlike many conventional pollutants, PFAS exhibit long biological half-lives and strong affinity for serum proteins, contributing to chronic exposure risks. Recent toxicological investigations associate PFAS exposure with immune modulation, endocrine disruption, hepatotoxicity, and certain malignancies. This review critically evaluates the structural characteristics influencing PFAS stability, pathways of environmental distribution, advances in ultra-trace analytical detection, and emerging destructive technologies including electrochemical oxidation, plasma-assisted degradation, and catalytic defluorination. Emphasis is placed on the technological limitations of current treatment systems and the urgent need for scalable mineralization strategies and regulatory harmonization. Future research directions toward sustainable PFAS mitigation are discussed.

Keywords: *PFAS, PFOA, PFOS, environmental persistence, advanced oxidation, electrochemical degradation, nanomaterials, remediation.*

Introduction

The rapid industrial expansion of fluorinated chemistry during the late twentieth century led to the development of per- and polyfluoroalkyl substances (PFAS), a broad family of synthetic compounds engineered for thermal stability, chemical resistance, and surfactant functionality. These materials have been incorporated into firefighting foams, polymer manufacturing, stain-resistant coatings, food-contact materials, and electronic components. The defining chemical feature of PFAS is the presence of multiple carbon–fluorine bonds, which are among the strongest covalent interactions in organic chemistry. This bond strength imparts remarkable resistance to hydrolysis, photolysis, and microbial degradation.

While these properties provide industrial advantages, they also prevent natural attenuation once PFAS enter environmental systems. Over the past decade, monitoring studies have confirmed their presence in groundwater aquifers, surface waters, polar ice, precipitation, and human blood serum across geographically distant regions. Such findings indicate extensive environmental mobility and long-range atmospheric transport. The persistence and bioaccumulative behavior of long-chain PFAS, combined with increasing evidence of adverse health effects, have positioned these compounds as contaminants of emerging global concern.

This review synthesizes recent advancements (2022–2025) in understanding PFAS chemistry, environmental fate, toxicological implications, detection technologies, and destruction strategies.

Chemical Structure and Physicochemical Properties

PFAS consist of a fully or partially fluorinated carbon chain attached to functional groups such as:

- Carboxylic acids (PFOA)
- Sulfonates (PFOS)
- Fluorotelomers Polyfluorinated precursors

Key Properties

Property	Significance
Strong C–F bond	Extreme chemical stability
Amphiphilic nature	Surfactant behavior
Hydrophobic & lipophobic	Bioaccumulation tendency
Thermal stability	Industrial applications

Long-chain PFAS (C8 and above) exhibit greater bioaccumulation, while short-chain PFAS are more mobile in aquatic systems.

Sources and Environmental Distribution

1. **Major Sources**

- Aqueous film-forming foams (AFFF)
- Fluoropolymer manufacturing
- Textile and leather treatment

2. **Environmental Pathways**

- Atmospheric transport
- Surface runoff
- Groundwater infiltration

Recent global rainfall studies (2022) indicate PFAS concentrations exceeding WHO drinking water guidelines in several regions.

3. **Toxicological and Ecological Impacts**

Recent epidemiological studies (2022–2024) link PFAS exposure to:

- Liver enzyme elevation
- Thyroid dysfunction
- Immune suppression

PFAS binds strongly to serum proteins rather than accumulating in adipose tissue, leading to long biological half-lives (2–8 years for PFOA/PFOS).

Ecologically, PFAS affect:

- Fish reproduction
- Bird immune systems
- Aquatic biodiversity

4. **Analytical Detection Methods**

Advanced detection techniques include:

- **LC-MS/MS (Liquid Chromatography–Tandem Mass Spectrometry)** – Gold standard
- High-resolution mass spectrometry (HRMS)
- Total oxidizable precursor (TOP) assay

Detection limits now reach parts-per-trillion (ppt) levels due to improved instrumentation (2023–2025 advancements).

Remediation Technologies

PFAS remediation remains challenging due to their resistance to degradation.

1. **Adsorption Technologies**

Material	Efficiency	Limitations
Activated carbon	Effective for long-chain PFAS	Less effective for short-chain
Ion exchange resins	High selectivity	Expensive regeneration
Biochar	Sustainable option	Lower capacity

Recent 2024 studies show modified biochar enhances short-chain PFAS removal.

2. **Advanced Oxidation Processes (AOPs)**

- UV–persulfate oxidation
- Photocatalysis (TiO_2-based systems)

Limitation: High energy requirement and incomplete mineralization.

3. **Electrochemical Degradation**

Electrochemical oxidation using boron-doped diamond (BDD) electrodes shows promising mineralization efficiency (up to 90%).

Electro-Fenton and anodic oxidation techniques demonstrate improved defluorination efficiency (2023 reports).

4. **Nanotechnology-Based Approaches**

- Graphene oxide composites
- Iron-based nanoparticles
- Silver nanoparticle-modified adsorbents
- Metal–organic frameworks (MOFs)

Nanomaterials enhance adsorption and catalytic breakdown but require toxicity evaluation.

Conclusion

PFAS contamination represents a critical environmental and public health challenge. Their chemical stability, while beneficial industrially, results in long-term ecological and biological persistence. Although significant advancements have been made in detection and remediation technologies between 2022 and 2025, large-scale and cost-effective mineralization solutions remain limited. Interdisciplinary collaboration among chemists, environmental scientists, policymakers, and engineers is essential for sustainable PFAS management.

Acknowledgment

The authors express their sincere gratitude to their respective institutions, Government Degree College, Ibrahimpatnam, and Government Degree College for Women (A), Nalgonda, for providing the necessary academic environment and facilities to carry out this work.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030110

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465566

DOI Link:
https://doi.org/10.5281/zenodo.19465566

Volume: 3

Issue: 1(I)

Pp. 49-52

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 10 Jan. 2026

Revised: 20 Jan. 2026

Accepted: 03 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
K. Anuradha. (2026). Diatom Diversity and Physico-Chemical Characteristics of a Freshwater Lake in Sangareddy District, Telangana, India. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 49–52.
https://doi.org/10.5281/zenodo.19465566

Diatom Diversity and Physico-Chemical Characteristics of a Freshwater Lake in Sangareddy District, Telangana, India

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Abstract

Diatoms are among the most sensitive biological indicators of freshwater ecosystem health due to their rapid response to environmental fluctuations. The present investigation evaluates diatom diversity in relation to selected physico-chemical parameters of a freshwater lake located in Sangareddy District, Telangana, India. Monthly sampling was carried out from January to December 2024 at three representative stations influenced by varying degrees of anthropogenic activity. A total of twelve diatom species belonging to six genera were recorded during the study period. Key water quality parameters including temperature, pH, dissolved oxygen, biochemical oxygen demand, nitrate, phosphate, silicate, sulphate and total dissolved solids were analyzed following standard methods. The results indicate moderate nutrient enrichment and declining water quality during summer and post-monsoon periods. The dominance of pollution-tolerant diatom species suggests increasing organic loading primarily from domestic wastewater discharge and agricultural runoff. The strong correlation between diatom assemblages and environmental variables confirms their effectiveness as bio-indicators of freshwater pollution. The study highlights the necessity of incorporating biological monitoring tools into lake conservation and management strategies for sustainable freshwater resource protection.

Keywords: *Diatom diversity, freshwater lake, water quality, bio-indicators, nutrient enrichment, Telangana*

Introduction

Conventional water quality monitoring primarily relies on physico-chemical parameters. While these provide instantaneous information, they often fail to reflect long-term ecological conditions (APHA, 2017). Biological communities, particularly microorganisms, offer a more integrative measure of environmental health. Among these, diatoms (Bacillariophyceae) are widely recognized as reliable bioindicators due to their sensitivity to nutrient concentration, pH, dissolved oxygen, and pollution levels (Patrick, 1977; Dixit et al., 1992).

Freshwater ecosystems play a crucial role in supporting biodiversity, maintaining ecological balance, and fulfilling human water requirements (Wetzel, 2001). Lakes serve as important reservoirs for drinking water, irrigation, fisheries, and recreational activities. However, increasing urbanization, agricultural intensification, and industrial development have significantly impacted water quality across many regions of India, resulting in eutrophication and biodiversity loss (Kelly & Whitton, 1995). Nutrient loading, organic pollution, and chemical contamination are major threats to freshwater bodies, resulting in eutrophication and loss of aquatic biodiversity.

Conventional water quality monitoring primarily relies on physico-chemical parameters. While these provide instantaneous information, they fail to reflect long-term ecological conditions. Biological communities, particularly microorganisms, offer a more integrative measure of environmental health. Among these, diatoms (Bacillariophyceae) are widely recognized as reliable bioindicators due to their sensitivity to changes in nutrient concentration, pH, dissolved oxygen, and pollution levels.

Diatoms respond rapidly to environmental stressors and display distinct species compositions under different water quality conditions (Round et al., 1990). Their siliceous cell walls allow preservation, enabling long-term ecological assessment. Numerous studies have demonstrated strong relationships between diatom assemblages and pollution gradients (Potapova & Charles, 2007; Wang et al., 2005).

In Telangana, freshwater lakes are increasingly subjected to anthropogenic pressures, particularly from urban sewage and agricultural runoff. Despite this, limited research has focused on diatom-based monitoring of lake ecosystems in the region. Therefore, the present study aims to assess diatom diversity in relation to physico-chemical parameters of a freshwater lake in Sangareddy District to evaluate its ecological status.

Objectives:

- To document diatom species diversity in the selected lake.
- To analyze seasonal variations in water quality parameters.
- To examine relationships between diatom assemblages and environmental conditions.
- To assess the pollution status of the lake using biological indicators

Study Area

The study was conducted in a freshwater lake located in sadasivpet, Sangareddy District, Telangana, India. The lake locally named as 'Vubbacheru' serves as a primary water source for nearby villages and supports agricultural activities. The region experiences a tropical climate with distinct summer, monsoon, and winter seasons. Average annual rainfall ranges between 750–900 mm, predominantly during the southwest monsoon.

Three sampling stations were selected based on surrounding land use patterns. Station, I represented relatively less disturbed conditions, Station II received moderate domestic wastewater input, while Station III was influenced by agricultural runoff and higher anthropogenic activities.

The lake exhibits shallow to moderate depth, with water levels fluctuating seasonally. The catchment area consists of cultivated lands, residential settlements, and small-scale commercial activities, contributing various pollutants into the lake system.

Materials and Methods

1. **Sample Collection**

Water and diatom samples were collected monthly from January to December 2024 from all three stations. Surface water samples were collected in clean polyethylene bottles for physico-chemical analysis. Water quality parameters were analyzed using standard methods recommended by the American Public Health Association (APHA, 2017).

Diatom samples were obtained by gently scraping submerged stones, aquatic plants, and sediments using a soft brush. Samples were preserved in 4% formalin for laboratory analysis. Diatom identification was carried out using standard taxonomic monographs (Round et al., 1990; Smol & Stoermer, 2010).

2. **Physico-Chemical Analysis**

Water quality parameters including temperature, pH, dissolved oxygen (DO), biochemical oxygen demand (BOD), nitrate, phosphate, silicate, sulphate, and total dissolved solids (TDS) were analyzed using standard methods recommended by the American Public Health Association.

Temperature and pH were measured in situ. DO was determined by Winkler's method, while BOD was estimated after five days of incubation. Nutrient concentrations were measured spectrophotometrically.

3. **Diatom Identification**

Preserved diatom samples were cleaned using acid digestion to remove organic matter and mounted on glass slides using DPX mountant. Identification was performed under a compound microscope using standard taxonomic keys and literature.

Species richness, abundance, and seasonal variation were recorded. Diatom assemblages were categorized based on pollution tolerance levels. Microphotographs were captured using a digital camera attached to a compound microscope. Image clarity was enhanced using standard contrast adjustment while maintaining original morphological features.

Results

1. **Physico-Chemical Characteristics**

Water temperature ranged from 22°C in winter to 34°C in summer. pH values remained slightly alkaline throughout the year, ranging between 7.2 and 8.6. Dissolved oxygen levels showed seasonal variation, with higher values during winter and lower levels during summer months.

BOD values increased significantly during post-monsoon and summer seasons, indicating organic pollution. Nutrient concentrations of nitrate and phosphate were elevated near Station II and Station III, particularly after monsoon runoff.

TDS values were higher during summer due to evaporation and concentration of dissolved salts.

2. **Diatom Diversity**

Plate I. Representative diatom taxa recorded from the freshwater lake in Sangareddy District (400× magnification). A total of twelve diatom species belonging to six genera were recorded. Dominant genera included Navicula, Nitzschia, Cymbella, Gomphonema, Pinnularia, and Fragilaria.

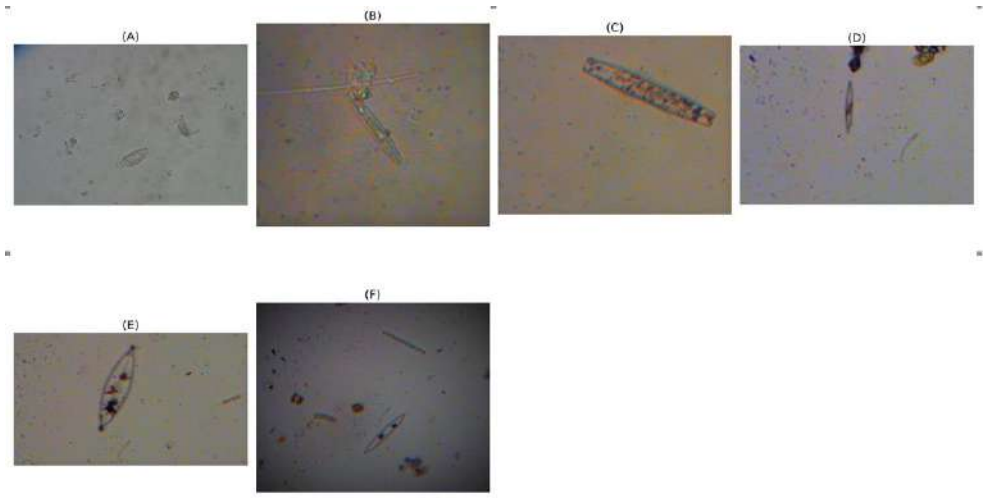
Pollution-tolerant species such as Nitzschia palea and Navicula cryptocephala were abundant at Station II and III. Relatively clean-water species were observed at Station I, particularly during winter months.

Seasonal variation revealed higher species diversity during winter and lower diversity during peak summer.

3. **Photographic Documentation of Diatom Taxa**

Plate I (A–G): Light microscopic photomicrographs (400× magnification) of dominant diatom species

All specimens were identified based on morphological characteristics following standard taxonomic monographs.



- Navicula cryptocephala — Elliptic-lanceolate valve with distinct raphe and central area.
- Gomphonema sp. — Clavate frustule with asymmetrical valve structure.
- Fragilaria sp. — Elongated rectangular form with parallel striae.
- Nitzschia palea — Linear-lanceolate valve with eccentric raphe system.
- Cymbella sp.—Dorsiventral, slightly curved valve.
- Pinnularia sp. — Broad elliptical valve with central nodule.

Discussion

The seasonal variation in physico-chemical parameters significantly influenced diatom assemblage structure. Elevated nitrate and phosphate concentrations during post-monsoon and summer periods promoted the dominance of eutrophic indicator species such as *Nitzschia palea* and *Navicula cryptocephala*. Similar nutrient-driven community shifts have been reported in tropical freshwater ecosystems (Kelly & Whitton, 1995; Potapova & Charles, 2007).

The presence of *Nitzschia* and *Navicula* species is commonly associated with organically polluted waters (Patrick, 1977; Dixit et al., 1992). Their dominance at stations receiving sewage and runoff confirms increasing anthropogenic pressure on the lake ecosystem.

The increased BOD values and reduced dissolved oxygen at Stations II and III indicate organic pollution stress, which favors pollution-tolerant taxa. The prevalence of *Nitzschia* species under such conditions corroborates findings of Wang et al. (2005) and Dixit et al. (1992), who reported their association with organically enriched waters.

Higher diversity during winter may be attributed to improved oxygen solubility and reduced thermal stress, consistent with observations in Indian tropical lakes (Bharati & Badola, 2018; Sharma & Singh, 2021). Seasonal recovery patterns suggest that the lake is currently in a moderately eutrophic state rather than severely degraded.

The strong correlation between diatom assemblages and environmental variables supports the application of diatom-based biomonitoring tools (Smol & Stoermer, 2010). Unlike instantaneous chemical measurements, diatom communities integrate environmental changes over time, providing a reliable ecological assessment (Wang et al., 2005). Unlike instantaneous chemical measurements, diatom communities integrate ecological conditions over time, providing a more reliable assessment of ecosystem health.

Overall, the increasing dominance of eutrophic indicator species signals early-stage ecological imbalance. Preventive nutrient management strategies are therefore critical to avoid progressive eutrophication.

The presence of Nitzschia and Navicula species is commonly associated with eutrophic and organically polluted waters. Their dominance at stations receiving sewage and runoff confirms increasing anthropogenic pressure on the lake ecosystem.

Higher diatom diversity during winter can be attributed to favorable temperature conditions, improved oxygen levels, and reduced nutrient stress. Similar seasonal patterns have been reported in other tropical freshwater ecosystems. The strong correlation between diatom assemblages and physico-chemical variables supports their use as reliable bioindicators for lake water quality assessment. Diatom-based monitoring provides a comprehensive ecological perspective beyond conventional chemical analysis.

Conclusion

The present study demonstrates that the freshwater lake in Sangareddy District is experiencing moderate nutrient enrichment and organic pollution, particularly in areas influenced by human activities. Diatom community composition effectively reflected variations in water quality, confirming their utility as sensitive bioindicators.

The increasing dominance of pollution-tolerant species signals the early stages of eutrophication, which may intensify if preventive measures are not implemented. Regular biological monitoring combined with pollution control strategies is essential for preserving freshwater ecosystem health. Effective wastewater management,

reduced agricultural chemical input, and community awareness programs are recommended to restore and protect the lake.

Acknowledgment
The authors express their sincere gratitude to their institution for providing the necessary facilities and support to carry out this research work. We are especially thankful to our respected supervisors and mentors for their constant guidance, encouragement, and valuable suggestions throughout the study.
We extend our appreciation to the laboratory staff and field assistants for their help during sample collection and analysis of physico-chemical parameters. Their cooperation was instrumental in the successful completion of this work.

Financial support and sponsorship
Nil.

Conflicts of interest
The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030111

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465658

DOI Link:
https://doi.org/10.5281/zenodo.19465658

Volume: 3

Issue: 1(I)

Pp. 53-56

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 12 Jan. 2026

Revised: 22 Jan. 2026

Accepted: 04 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
L. Kamala. (2026). New Vistas of Chemistry—An Interdisciplinary Approach: Phyto-Mediated Synthesis of Silver Nano-Particles (AgNPs). International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 53–56.
https://doi.org/10.5281/zenodo.19465658

New Vistas of Chemistry—An Interdisciplinary Approach: Phyto-Mediated Synthesis of Silver Nano-Particles (AgNPs)

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Abstract

With the advent of the 21st century, chemical sciences have taken a broad, humane turn in going through a radical redefinition and reorientation from an age-old, classical, and rather rigid compartmentalized paradigm into that of interdisciplinary convergence. This report marshals the exhaustive account of phyto-assisted production of silver nanoparticles (AgNPs) from Azadirachta indica (Neem) as a case study where botany, surface chemistry, quantum physics, and microbiology transfer seamlessly into one another. In this eco-friendly, single-step process, phytochemicals such as terpenoids, flavonoids, or reducing sugars in plants will act reductively, whereby silver ions (Ag^{+}) will be reduced to metallic silver (Ag^{0}) and stable in a subsequent step. Optimization studies suggest that neutral pH (pH 7) and 75 ºC are the most ideal conditions for maximizing the yield and size homogeneity of AgNPs produced. The results of physicochemical characterization through UV-Visible spectroscopy yield a clear-cut Surface Plasmon Resonance (SPR) peak in the 400-420 nm range, while XRD studies confirm a cubic crystal structure with the average size of the crystallite ranging between 1 and ~30 nm.

FTIR spectrometry gives direct evidence of the 'protein corona' formed by amide and carbonyls contributed from plant metabolites that hold the particles in space by steric hindrance Physicochemical characterization through UV-Visible spectroscopy shows a distinct peak of Surface Plasmon Resonance (SPR) in the range of 400-420 nm, while analysis of XRD confirmed a Face-Centered Cubic (FCC) crystalline structure with average crystallite sizes between 10 and 30 nm. FTIR spectroscopy provides direct evidence of a "protein corona," which is a condition in which amide and carbonyl groups from plant metabolites stabilize the particles through steric hindrance. Biological evaluation shows that it has broad-spectrum antimicrobial action with special reference to Gram-negative Escherichia coli (ZOI ~17 mm), acting via membrane-disrupting oxidative stress pathways. The other significant advantage of these AgNPs is that they are highly potent in environmental remediation, achieving efficiency greater than 90% in the catalytic degradation of organic dye molecules while providing very sensitive colorimetric sensing for heavy metals like mercury and lead. This inter-disciplinary process constitutes a highly scalable, robust technology that promises to overcome global challenges in healthcare and sustainability.

Keywords: *Green Chemistry, Azadirachta indica, Silver Nanoparticles, Phyto-reduction, Antimicrobial Activity.*

Introduction

The twenty-first century is a transformative period in chemical sciences, characterized by the transition from classical and rigid compartmentalization to fluid, interdisciplinary convergence. The most salient expressions of this "New Vista" are found in the emerging field of nanobiotechnology, where the precision of inorganic chemistry meets the complexity of biological systems. The report describes in detail the phyto-mediated synthesis of silver nanoparticles (AgNPs) using Azadirachta indica (Neem), presenting a case study embodying the seamless integration of botany, surface chemistry, quantum physics, and microbiology.

The formation of metal nanoparticles, such as silver, traditionally been the domain of physical and chemical metallurgy. Conventional processes of laser ablation, vacuum sputtering, or softer types of chemical reduction by sodium borohydride ($NaBH_4$), or hydrazine (N_2H_4), have the ability to generate nanoparticles of a well-defined geometry. These "top-down" and chemical "bottom-up" approaches, however, impose a heavy environmental debt. They consume enormous amounts of energy, rely on hazardous organic solvents, and produce toxic effluents whose disposal becomes an expensive proposition. In addition, nanoparticles synthesized by chemical routes require the addition of synthetic stabilizing agents (capping agents) such as polyvinylpyrrolidone (PVP) or citrate to prevent agglomeration, which, however, could compromise their biocompatibility in medical applications.

To meet these challenges, the scientific world has adopted the principles of Green Chemistry. This encompasses a view of the design of chemical products and processes to minimize or eliminate the production and use of hazardous substances. In this sense, the use of plant extracts as "bio-factories" for the synthesis of nanoparticles has been viewed as an excellent alternative.

The potent Azadirachta indica tree, native to the Indian sub-continent, is highly praised by Ayurveda with the epithet of "village pharmacy" and contains a variety of phytochemicals that make this plant a good candidate for this biosynthetic pathway. With the help of the reducing power of the phytochemicals-terpenoids, flavonoids, and reducing sugars, the reduction of silver ions (Ag^{+}) to metallic silver (Ag^{0}), closely followed by stabilization, can be achieved in a single green step.

The report "New Vistas of Chemistry" examines this interdisciplinary framework in minute detail. It expounds upon the theoretical basis of green synthesis, discusses thermodynamic and kinetic optimization of the reaction, describes physicochemical characterization of produced nanomaterials, and evaluates their applications in areas such as antimicrobial therapy and environmental remediation. In this thorough examination, it has been shown that the phyto-mediated synthesis of AgNPs is not just an attractive new idea for laboratory work, but a robust and scalable technology that can be poised to face very real challenges in global health and environmental sustainability.

Experimental / Methodology

The synthesis of AgNPs via *Azadirachta indica* is grounded in the "12 Principles of Green Chemistry," a set of guidelines formulated to minimize the environmental impact of chemical manufacturing.

1. **Preparation of Plant Extract**

The leaf extract of Azadirachta indica is constituted of an array of bioactive compounds. Qualitative and quantitative screenings have led to the identification of many classes of metabolites of paramount importance in the synthesis of nanoparticles: Flavonoids, including quercetin and rutin, are potent antioxidants bearing free hydroxyl (-OH) groups on the aromatic ring. The oxidation of these hydroxyls onto keto structures liberates electrons that will be able to reduce metal ions. Terpenoids, including limonoids, azadirachtin, and nimbin, assist in the reduction and also hold a key position in surface stabilization of nanoparticles, given their bulky steric nature. Simple carbohydrates present in the extract mildly reduce and somehow initiate the nucleation process. Proteins in the extract with functional groups including amines, carboxylic acids, and thiols will bind to the silver surface, forming what can be termed the 'protein corona'.

2. **Synthesis of Silver Nanoparticles (AgNPs)**

Referred to as the transition from chaotic ions into a monodispersed dispersion of nanoparticles, this is achieved via proper control of the reaction kinetics. AgNP characteristics such as size, shape, and yield are strictly determined by pH, temperature, and reactant concentration, among other factors.

- **pH Optimization:** A neutral pH (pH 7) or slightly acidic pH (pH 6) is optimal for synthesizing stable AgNPs with Azadirachta indica. At neutral pH, the ionization of phenolic and carboxylic acid groups in the extract is balanced, facilitating strong coordination with Ag^{+} ions.
- **Temperature Optimization:** Studies suggest that a temperature of approximately 75°C yields the maximum production of uniform AgNPs. Increasing the temperature to 75°C accelerates the reduction rate, leading to a "burst nucleation" event where many nuclei form simultaneously.
- **Reactant Concentration:** An optimized concentration of 1 mM $AgNO_3$ is consistently cited as ideal. A volume ratio of approximately 3:7 (Extract: Nitrate Solution) has been identified as effective

3. **Characterization Techniques**

The successful synthesis of AgNPs is validated through a suite of advanced characterization techniques:

- **UV-Visible Spectroscopy:** Used to monitor Surface Plasmon Resonance (SPR).
- **Fourier Transform Infrared Spectroscopy (FTIR):** Used to identify specific phytochemicals involved in reduction and capping.
- **X-Ray Diffraction (XRD):** Used to confirm the crystalline nature of the material.
- **Transmission Electron Microscopy (TEM):** Used for direct visualization of nanoparticle morphology and size.
- **Zeta Potential:** Used to measure the effective surface charge for colloidal stability analysis.

Results & Discussion

1. **UV-Visible Spectroscopy:**

The Surface Plasmon Resonance:

The interaction between silver nanoparticles and light through Surface Plasmon Resonance (SPR) is the primary signature. Neem-mediated AgNPs showed a consistent absorption peak in the region of 400-420 nm. The appearance of the peak at ~400 nm corresponds to roughly 10-20 nm spherical particles. The intensity of the peak is proportional to the concentration of nanoparticles in the solution. Silver nanoparticles basically echo their qualities in interaction with light through Surface Plasmon Resonance (SPR). In the case of Neem mediated AgNPs, a typical absorption peak always falls between 400-420 nm with a specific absorption peak at ~400 nm related to spherical particle size ranging 10-20 nm. The intensity of the peak is directly related to the concentration of nanoparticles in the solution.

2. **Fourier Transform Infrared Spectroscopy (FTIR)**

FTIR spectroscopy gives a molecular fingerprint of the nanoparticle surface. The analysis showed strong bands at ~1634 cm^{-1} and ~1602 cm^{-1} in purified AgNPs. These bands confirm the attachment of amide groups from proteins and carbonyl groups of flavonoids on the silver surface, providing direct spectroscopic evidence for the "protein corona" theory. The O-H Stretching bands observed in the region of 3200-3480 cm^{-1} are an indication of the involvement of polyphenols and flavonoids in the reduction process.

3. **X-Ray Diffraction (XRD)**

XRD investigation certainly confirmed the formation and crystalline nature of the synthesized material. Neem-mediated AgNPs exhibit a face-centered cubic (FCC) lattice structure. The major diffraction peaks are generally located at around 2θ values of 38°, 44°, 64°, and 77°, respectively, corresponding to (111), (200), (220), and (311) crystallographic planes. Studies consistently report average crystallite sizes from 10 to 30 nm.

4. **Morphology and Size (TEM)**

It's evident from the Transmission Electron Microscope (TEM) characterizations that the morphology is almost spherical. The size distribution, like all silver nanocolloids, is polydisperse, having diameters generally from about 10 to 43 nm, but such a distribution is considerably reduced to having average sizes close to 12 nm under optimized conditions (pH 7, 75 C). Micrographs typically show fairly well-dispersed particles with few agglomerations.

5. **Antimicrobial Efficacy**

AgNPs synthesized via *Azadirachta indica* exhibit broad-spectrum antimicrobial activity. A comparative analysis reveals distinct patterns of susceptibility:

- **Escherichia coli (Gram-Negative):** AgNPs show a Zone of Inhibition (ZOI) of ~17 mm. Gram-negative bacteria are generally more susceptible due to their thinner peptidoglycan layer (~7-8 nm) and the presence of negatively charged lipopolysaccharides (LPS) that attract positively charged AgNPs.
- **Staphylococcus aureus (Gram-Positive):** AgNPs show a ZOI of ~16 mm. The thick, rigid peptidoglycan layer (20-80 nm) of Gram-positive bacteria acts as a robust physical barrier.

The modes of action of AgNPs with respect to bactericidal activity include causing "pits" on the surface of the cell wall, which leads to leakage, inducing the generation of Reactive Oxygen Species (ROS) responsible for oxidative stress, and releasing silver ions that inhibit respiratory enzymes.

6. **Environmental Applications**

- **Catalytic Degradation:** Neem-mediated AgNPs exhibit remarkable catalytic activity in degrading azo dyes like Methylene Blue (MB). Under optimized conditions (pH 2.0), degradation efficiencies of >90% have been achieved within 24 hours. The process is photocatalytic and significantly accelerates under sunlight.
- **Heavy Metal Sensing:** AgNPs can serve as optical sensors for heavy metals. When ions like Hg^{2+} or Pb^{2+} are added, they interact with capping agents, causing aggregation and a visible color change. Detection limits as low as 16 nM for Mercury have been reported.

Conclusion

The "New Vistas of Chemistry" are defined by the convergence of disciplines. The synthesis of Silver Nanoparticles using Azadirachta indica is a quintessential example of this convergence, merging ancient ethnobotanical knowledge with cutting-edge nano chemistry. By optimizing key parameters like pH and temperature, and by leveraging the complex phytochemical matrix of Neem, researchers have developed a synthesis route that is not only green and sustainable but also yields nanomaterials with potent antimicrobial and catalytic properties. As we overcome the hurdles of standardization, these "green" nanoparticles stand poised to revolutionize fields ranging from infectious disease management to environmental remediation.

Acknowledgment

The authors express their sincere gratitude to all those who contributed to the successful completion of this work. We are especially thankful to our institution for providing the necessary facilities, infrastructure, and academic support to carry out this research.

We extend our heartfelt appreciation to our supervisors and mentors for their invaluable guidance, constant encouragement, and insightful suggestions throughout the course of this study. Their expertise greatly enhanced the quality of this work.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030112

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465741

DOI Link:
https://doi.org/10.5281/zenodo.19465741

Volume: 3

Issue: 1(I)

Pp. 57-60

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 12 Jan. 2026

Revised: 22 Jan. 2026

Accepted: 04 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Prameela, K. L., & K. Anusha. (2026). Applications of Nanotechnology for Environmental Remediation. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 57–60.
https://doi.org/10.5281/zenodo.19465741

Applications of Nanotechnology for Environmental Remediation

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Abstract

One of the most pivotal challenges faced by the ultramodern world moment is environmental pollution performing from ever- growing urbanization, deforestation, and industrialization. Different adulterants, like diseases, poisonous colorings, heavy essence, inorganic and organic composites and artificial backwaters, affect all major environmental factors, including water, soil, and air. Several strategies like adsorption, filtration, aerobic/ anaerobic digestion, coagulation, natural pollutants, actuated sludge, chemical rush, photocatalysis, and advanced oxidation processes with different strategies are being delved for the requital of these pollutants from the terrain. Nanotechnology- grounded ways have been reported to be more effective and effective in environmental remediation. Research into physical and natural chemistry revision by masterminds and scientists to produce new accoutrements with asked morphology that can exclude a variety of environmentally dangerous adulterants is still ongoing. These accoutrements aim to use minimum energy, reduce cost, and achieve optimal performance. For effective environmental remediation, acceptable care is demanded to avoid using accoutrements that produce secondary or intermediate adulterants. This has led to the wide use of nanomaterials deduced from sustainable and biodegradable sources as an effective environmental remediation in the field of nanoscience. Through incubating exploration, diving safety enterprises, and promoting interdisciplinary collaboration, nanotechnology will come a crucial asset in restoring our earth to its natural state so that all unborn life may flourish.

Keywords: *Nanotechnology, Fundamentals of Nanotechnology, Environmental Remediation*

Introduction

One of the most pivotal challenges faced by the ultramodern world moment is environmental pollution performing from ever- growing urbanization, deforestation, and industrialization. Different adulterants, like diseases, poisonous colorings, heavy essence, inorganic and organic composites and artificial backwaters, affect all major environmental factors, including water, soil, and air. Several strategies like adsorption, filtration, aerobic/ anaerobic digestion, coagulation, natural pollutants, actuated sludge, chemical rush, photocatalysis, and advanced oxidation processes with different strategies are being delved for the requital of these pollutants from the terrain. Nanotechnology- grounded ways have been reported to be more effective and effective in environmental remediation. Research into physical and natural chemistry revision by masterminds and scientists to produce new accoutrements with asked morphology that can exclude a variety of environmentally dangerous adulterants is still ongoing. These accoutrements aim to use minimum energy, reduce cost, and achieve optimal performance. The development of new nanomaterials for environmental remediation faces the crucial challenges of the sustainable conflation system, nontoxicity, recovering capability, rejuvenescence capability, biodegradability, and more basically, sustainability. Understanding colorful types of nanomaterials used for soil, water, or air recovery as well as their manufacturing process with reference source accoutrements like shops, is essential to relating sustainable nanotechnology- grounded approaches for environmental remediation. This paper aims to probe and assess the capacity of nanotechnology as a feasible and effective system for delivering environmental remediation, targeting different types of environmental pollutants, and enhancing the cleanliness and safety of ecosystems.

Fundamentals of nanotechnology:

Nanomaterials similar as nanorods, nanotubes, nanofibers, nanoparticles, nanoplates, and carbon- grounded nanomaterials have excellent mechanical, optic, thermal, and electrical parcels and performance for different operations, including environmental remediation, due to their nanoscale size. Nanocomposites are a combination of nanoparticles (mounts or paddings) and a matrix (a structure with a nonstop phase in which the nanoparticles are immersed) of bulk accoutrements like polymers and pottery, which improves the base material's property performance.

The nanoparticles are a dispersed phase that gives the nanocomposite unique characteristics. These nanocomposite accoutrements parade enhanced mechanical performance, bettered continuity and hardness with better heat resistance, hedge parcels, and thermal conductivity. Composite accoutrements have a wide range of engineering operations. Nanostructured accoutrements have a larger viscosity of reactive spots on their flyspeck shells due to their high face area, which increases their overall effectiveness and high rate of decontamination. Subject to the area of operation and conditions, nanomaterials' performance parcels through a design, picky, and controlled conflation approach can be bettered. The face of finagled nanomaterials is functionalized to enable targeted relations with target motes or pollutants for effective environmental remediation. mongrel mixes with asked performance parcels present possible and more effective and stable nanomaterials for environmental remediation than single- type nanoparticles approach. Grounded on their mode of action, the nanoparticles (NPs) employed in environmental remediation can be distributed as reactive nanomaterials and nano- adsorbents. These types of nanomaterials work through chemical processes like redox, acid- base, rush, photocatalysis, and catalysis.

Applications of Nanotechnology for Environmental Remediation

Water/ wastewater remediation: One of the most remarkable features of the world is water, which is largely significant to the actuality of life. Although the globe is girdled by water, only 2.5% of the world's water is brackish. In polar regions, over 70% of freshwater is firmed, and the remaining significant quantum is present either in deep aquifers or as humidity that's inapproachable to humans. Still, only 1% of all freshwater is fit for mortal use, pressing how vital water is to life. A many decades ago, water, was a natural resource that was free and accessible, but owing to unbridled recessions, overuse, and inordinate impurity of water coffers, the world is presently passing a severe water extremity. Remediation of water from colorful dangerous substances, like colorings, heavy essence, and medicinals, is greatly demanded to control this impurity of the water terrain. numerous experimenters have employed traditional styles with colorful accoutrements, including biochar deduced from colorful sources, actuated carbon, and colorful low- cost adsorbents for water remediation. Nanostructured accoutrements have entered adding interest in the field of water and wastewater recovery because of their exceptional rates and bettered performance. Several experimenters have delved and reported that nanomaterials hold great eventuality in adsorbing and/ or demeaning a variety of pollutants from the air, soil, water, and wastewater, including heavy essence, medicinals, and colorings. colorful nanomaterials have been linked as promising options for environmental remediation, including nanomembranes, nanocatalysts, and nano- adsorbents.

Nano- adsorbents: Nanoparticles are significantly employed as feasible adsorbents because of their larger face area and comparatively reduced mass. kinds of nano- adsorbents are used, including manganese oxide, actuated carbon, graphene, titanium and ferric oxides, carbon nanotubes (CNTs), and actuated carbon. Nanomaterials have dynamic parcels due to their ingrain face and varied external functionalization. The nanoparticles have proven to be perfect adsorbents because of their essential composition, foreign structure, and apparent size. colorful characteristics may have an impact on the nanomaterials employed to remove colorings, heavy essence, and other pollutants from the submarine terrain. It's important to note that the nanomaterials should be nontoxic, have a advanced adsorption capacity, be effective indeed at low attention of adulterants, and allow for easy separation of the adulterants from their face following treatment. Depending on their adsorption capacity, NPs can take numerous different forms. These include glamorous, metallic, and nanostructured mixed oxide NPs. In recent times, experimenters have been in the product and application of carbonaceous nanomaterials, similar as carbon nanoparticles, carbon nanosheets, and carbon nanoparticles, as adsorbents. It has also been reported that silicon nanomaterials, similar as silicon NPs, silicon nanotubes, and silicon nanosheets, are being used as adsorbents for environmental remediation. Aerogels, nanofibers, and nanoclays are among other nano- adsorbents that are used for the junking of heavy essence from waterless results and be paint adsorption.

Nanocatalysts: Inorganic nanomaterials like semiconductors and essence oxides are gaining significant interest for use as catalysts in wastewater treatments. For use in wastewater recovery, different types of nanocatalysts have been reported, including electrocatalysts, photocatalysts, and Fenton- grounded catalysts for chemical oxidation and antibacterial conditioning. Nanocatalysts are NPs that parade a photocatalytic response when exposed to light. They can be used in wastewater to reduce a variety of poisons in a wide range of operations. To breakdown pollutants including heavy essence, cleansers, fungicide colorings, and other substances set up in wastewater, these photocatalysts are made of semiconductor essence.

Nanomembranes: One of the stylish ways for wastewater treatment is nanomembrane filtration processes. The catalytic reactivity, profitable viability, high permeability, high effectiveness, water quality, fouling resistance, effective disinfection, and ease of design due to the drinkable filtration factory size make the operation of nanomembrane filtration an excellent approach for environmental remediation. Successful and effective junking of inorganic and organic pollutants through membrane filtration including colorings and heavy essence from wastewater for a cleanser terrain.

Nanotechnology- supported soil pollution remediation: Another essential element of the terrain, demanded to sustain life on Earth is the soil which is the only means of food product and factory growth. Maintaining healthy soil is essential for conserving environmental balance and guarding agrarian productivity. The world is faced with the adding challenge of environmental deforestation, soil corrosion, urbanization, etc., performing in soil impurity and declination which need critical attention. This soil impurity is also caused by the presence of a variety of chemical pollutants in the soil. Thus, environmental remediation is urgently demanded for healthy living. Nanotechnology holds enormous implicit for use in soil remediation, analogous to the treatment and recovery of water and

wastewater. Several nanomaterials like CNTs, nano- zero- valent iron(nZVI), and titanium dioxide (TiO2) have been reported as excellent nanomaterials for environmental soil remediation.

The success history of nanotechnology- grounded ways is attributed to their malleable nature and the unique parcels of certain pollutants, and this makes them far more suited for soil remediation. Nano- zero- valent iron has been reported as an excellent nanomaterial for the reduction of Zn, Pb, Cr, and Cd in amalgamation- defiled soil alongside sustainable stabilizers like carboxymethyl cellulose (CMC) and bounce as soil remediation. Nanocomposites are excellent accoutrements for arsenic junking from polluted soil. The nanoparticles suffer a response process where chemical adulterants are converted to inoffensive substances. The chemical pollution response in this case changes the composites in the dangerous fungicides into safe adulterants. Titanium dioxide and zinc oxide are regarded as effective soil remediation photocatalysts. Soil quality is bettered by the use of nanomaterials- grounded detectors or nanosensors performing in increased crop productivity. In artificial units, nanosensors identify and cover dangerous adulterants, dressings, etc. Both the discovery of fungicide residue and the wide range of soil quality can be greatly enhanced by nanosensors.

Air pollution remediation through nanotechnology:

Air pollution is a global challenge involving dust, heavy essence, feasts, and other patches due to colourful mortal- caused factors. Air pollution remediation and control are extremely important and are seen as ultramodern-day musts. Consequently, styles grounded on nanotechnology are essential for the discovery, treatment and control/ forestalment of air pollution. These styles include the use of nano- adsorbents for the adsorption of air adulterants, Nano catalysts to degrade pollutants, and Nano membranes for contaminant separation. Several dimensional nanos-adsorbents, including carbon nanotubes (CNTs), fullerene, graphite, and grapheme have been reported for use as air pollution remediation.

Carbon dioxide and other hothouse feasts are constantly emitted into the atmosphere in a variety of ways, and they've dangerous impacts on the ecosystem. Nanotechnology- grounded approaches have proven excellent and easy results to state pollution remediation. Nano- adsorbents have a high degree of hydrophobic, hydrogen bond, pie- pie, electrostatic, and van der Waals forces with organic motes. The spherical pores held by CNTs make them excellent adsorbents over actuated carbon. Titanium oxide nanoparticles (NPs) retain a tone- drawing coating that helps remove gassy adulterants and other air adulterants including nitrogen oxides. Nanofiber- carpeted sludge medium has proven an excellent air cleaner for artificial factory air input and turbine bay air. The identification of different air adulterants in an terrain is a critical first step in the control of air pollution.

Conclusion:

Exercising nanotechnology to address some of the most delicate problems in the world of environmental remediation is gaining significant interest among experimenters. Because of their large face area, reactivity, and the possibility to mastermind them at infinitesimal scale; nanomaterials were well suited for pollution junking from water, soil, or air. This technology makes the design of more effective, cheaper, and sustainable remediation styles possible compared to traditional ways. The targeting of some particular adulterants with high delicacy is one of the significant benefits that nanotechnology provides for environmental remediation. For illustration, nanoparticles like nano zero- valent iron (nZVI) can degrade/ transfigure poisonous heavy essence and organic pollutants in groundwater to a lower dangerous state. Nanotechnology serves as a sustainable and important delivery system for environmental remediation. The fact that it can increase pollution control and measure both its effectiveness and effectiveness makes climate change an important motorist of unborn environmental sustainability. Through incubating exploration, diving safety enterprises, and promoting interdisciplinary collaboration, nanotechnology will come a crucial asset in restoring our earth to its natural state so that all unborn life may flourish.

Acknowledgment

The authors express their sincere gratitude to their institution for providing the necessary facilities, resources, and a conducive environment for carrying out this study. We are deeply thankful to our supervisors and mentors for their constant guidance, valuable insights, and encouragement throughout the preparation of this work.

We also acknowledge the contributions of researchers and scientists whose published studies in the field of nanotechnology and environmental remediation have significantly supported this review. Their work has been instrumental in shaping our understanding of the subject.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| *Volume-3 Issue-1(I)* | *February-2026* | *ISSN: 3066-0637* | *Website:* https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030113

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465806

DOI Link: https://doi.org/10.5281/zenodo.19465806

Volume: 3

Issue: 1(I)

Pp. 61-64

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 12 Jan. 2026

Revised: 22 Jan. 2026

Accepted: 04 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
M. Prabhavathi, & Panda, S. (2026). Biophysical Characterization of Drug–Protein Interactions through UV, Fluorescence, and Circular Dichroism Spectroscopy. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 61–64. https://doi.org/10.5281/zenodo.19465806

Biophysical Characterization of Drug-Protein Interactions through UV, Fluorescence, and Circular Dichroism Spectroscopy

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Abstract

Understanding drug–protein interactions is critical for predicting pharmacokinetics and therapeutic performance. This study investigates the interaction between Favipiravir (FAV) and human hemoglobin (HHb) using UV–Visible absorption, fluorescence quenching, and circular dichroism (CD) spectroscopy. UV–Vis spectra revealed hyperchromicity with a slight red shift in the Soret band, indicating ground-state complex formation. Fluorescence quenching analysis confirmed a static mechanism with moderate binding affinity ($Kb \approx 3.2 \times 10^4\ M^{-1}$ at 298 K) and 1:1 stoichiometry. Thermodynamic parameters ($\Delta H° < 0$, $\Delta S° < 0$) suggest hydrogen bonding and van der Waals forces dominate the interaction. CD analysis showed a small decrease in α-helical content (72.0% → 68.1%), confirming minor conformational adjustments without denaturation. The integrated spectroscopic approach provides a reliable framework for elucidating drug–protein binding mechanisms relevant to drug design and pharmacokinetic prediction.

Keywords: *Drug–protein interaction, Human hemoglobin, Favipiravir, Fluorescence quenching, Circular dichroism, Thermodynamics.*

Introduction

Pharmacology relies on drug–protein interactions to control drug bioavailability, metabolism, excretion, and toxicity [1]. An undoable drug binding to plasma proteins occurs in the blood. The main carriers are HSA and Hb. A tetrameric heme-protein that delivers oxygen, hemoglobin binds strongly to numerous substances, including medicines [2]. Strong, label-free, solution-phase spectroscopic technologies allow us to study these molecular interactions in body-like settings. Each technique provides different data: UV–Visible absorption spectroscopy detects microenvironmental changes and complexity around chromophores. Fluorescence quenching spectroscopy determined binding constants, stoichiometry, and quenching mechanisms [3]. Protein secondary and tertiary structure can be detected using CD spectroscopy [4]. This multi-technique approach avoids the drawbacks of any single method and gives us a multifaceted knowledge of the interaction.

This study examines the interaction between a model pharmacological molecule and human hemoglobin using UV–Visible, fluorescence, and CD spectroscopy. The objectives are to (i) confirm a drug–Hb complex, (ii) determine the binding strength and number of molecules, (iii) determine the strongest intermolecular forces, and (iv) determine if the drug modifies protein structure. The goal of this interdisciplinary biophysical analysis is to anticipate in vivo behavior and improve treatment efficacy.

Materials and Methods:

Materials:

Human hemoglobin (Sigma-Aldrich) and analytical-grade chemicals were used. A 20 mM phosphate buffer (pH 7.4) simulated physiological conditions.

Measurements with Spectroscopy

1. **UV–Visible Absorption Spectroscopy**

Shimadzu UV-2600i spectrophotometer used to record absorption spectra. Scans were done between 250 and 500 nm. Spectral changes including shifts in wavelength (λmax) and changes in absorbance were analysed as evidence of complex formation and alterations in the chromophore's environment [6].

2. **Spectroscopy of Fluorescence Quenching**

Fluorescence spectral studies of interaction of IVM and HHb were carried out using a HITACHI F-2700 spectrofluorometer equipped with a 1 cm quartz cuvette. Hb was excited at 280 nm, and the emission spectrum was recorded from 300 to 450 nm. Inner filter effects were corrected using the standard formula [3].

3. Circular Dichroism (CD) Spectroscopy

Spectra were acquired on a Jasco-1500 spectropolarimeter equipped with a 0.2 cm path-length cuvette over the range of 190-240 nm. The mean residue ellipticity (MRE) was calculated, and the α-helical content was estimated from the MRE value at 222 nm [4, 10].

Results and Discussion

1. UV–Visible Absorption Spectroscopy Analysis

The UV–Vis spectra of natural Hb showed a large Soret band [5] at 406 nm and a lesser one at 278. After adding the drug incrementally, the Soret band became hyperchromic and redshifted by 2–3 nm. These findings suggest a ground-state complex between Favipiravir and Hb [6, 11]. The hyperchromicity shows that drug binding modifies the $\pi \rightarrow \pi^*$ transitions of the heme porphyrin ring, presumably due to microenvironment polarity alterations. The red shift suggests a modest decrease in transition energy, which is commonly linked to heme pocket conformational stress [12].

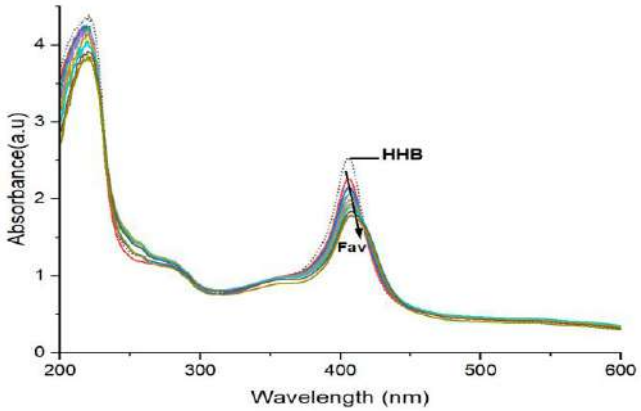


Fig:1 Absorption spectra of pure HHb (2 μM) (top dotted line) and with consecutive addition of Fav (0 to 10 μM)

2. Fluorescence Quenching and Binding Parameters

HHb has strong intrinsic fluorescence because it has tryptophan residues. The fluorescence intensity at approximately 335 nm diminished progressively with escalating drug concentration (Fig. 2), signifying effective quenching.

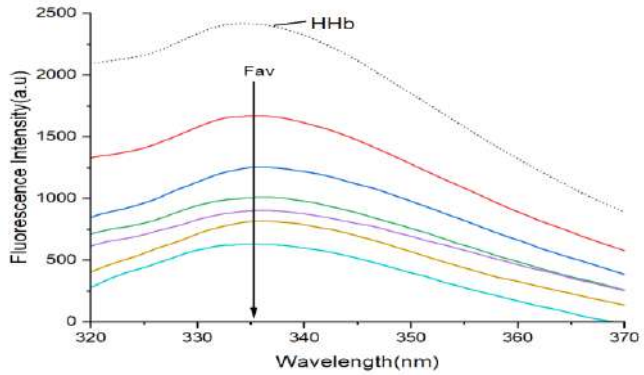


Fig. 2 Emission spectra of pure HHb (1 μM) (top dotted line) and with FAV (0-10 μM; solid lines);

Arrow is an indication of quenching with rise in the [FAV]

The Stern-Volmer figure indicated a straight line at lower concentrations, whereas K values decreased with increasing temperature. This inverse temperature dependence characterizes static quenching [7, 13]. The bimolecular quenching constant k was significantly larger than the highest diffusion-controlled collision constant, supporting static quenching [8].

The double-logarithmic plot showed a linear fit, indicating a binding constant K_a of 3.2×10^4 M^{-1} at 298 K and a site number n approaching 1. According to studies on similar drug-Hb systems [14], this indicates a moderate binding affinity with 1:1 stoichiometry

3. Thermodynamic Analysis and Binding Forces

The temperature-dependent binding constants were used to determine thermodynamic parameters (Table 2). The values of ΔG were negative, confirming spontaneity. Both ΔH^0 and ΔS^0 were found to be negative.

According to Ross and Subramanian's theory, negative $\Delta H^{o}$and ΔS^{o}values are typical for interactions dominated by hydrogen bonding and van der Waals forces in an enthalpy-driven process [9, 15]. This suggests that the drug binds to a polar region of Hb, forming specific hydrogen bonds.

Table 2: Thermodynamic parameters:

T (K)	Kb ± SD ($\times 10^4$ M^{-1})	ΔG° ± SD (kJ/mol)	ΔH° ± SD (kJ/mol)	ΔS° ± SD (J/mol·K)
298	3.20 ± 0.05	-25.70 ± 0.10	-37.37± 12.0	-39.9 ± 40.4
303	2.85 ± 0.12	-25.83 ± 0.10		
308	1.95 ± 0.15	-25.26 ± 0.10		

4. **Circular Dichroism: Conformational Stability Assessment**

In the far-UV CD spectra of natural Hb, negative bands at 208 and 222 nm indicate a significant α-helical concentration. As seen in Fig. 3, drug (Fav) binding retained the spectrum's overall shape, showing the protein's global fold [16]. In contrast, negative ellipticity decreased little. In Table.3, quantitative analysis showed a drop in α-helical content from 72.01 to 68.1%. The medication causes localized structural changes with this little reduction [10, 17]. The shift is mild, confirming a non-denaturing interaction.

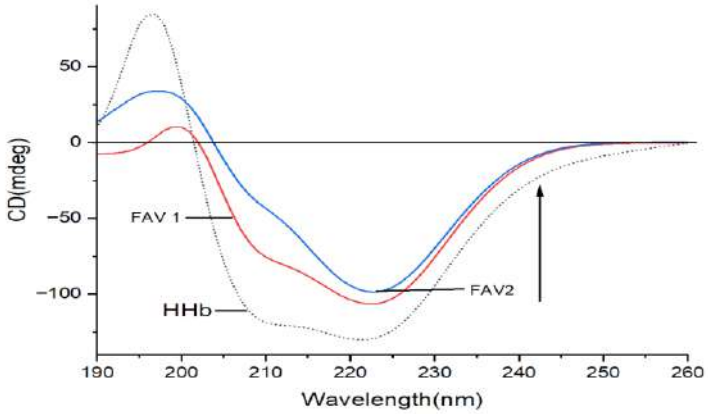


Fig. 3: CD spectra of HHb (dotted line) and HHb in presence of FAV at different molar ratios (solid line)

Conclusion

The interaction between FAV and human hemoglobin (HHb) was comprehensively investigated using biophysical techniques and molecular docking. UV-Vis and fluorescence spectroscopy provided qualitative evidence of FAV binding to HHb. Thermodynamic analysis at three different temperatures demonstrated that the interaction is dynamic, spontaneous, and driven primarily by entropy. Structural changes induced by FAV binding were confirmed through Circular dichroism spectroscopy.

Acknowledgment

The authors express their sincere gratitude to their institution for providing the necessary facilities, instrumentation, and a supportive research environment to carry out this work. We are deeply thankful to our supervisors and mentors for their constant guidance, valuable insights, and encouragement throughout the course of this study.

We extend our appreciation to the laboratory staff and technical personnel for their assistance in spectroscopic measurements and data analysis, particularly in UV–Visible, fluorescence, and circular dichroism studies. Their expertise and support were essential for the successful completion of this research.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| *Volume-3 Issue-1(I)* | *February-2026* | *ISSN: 3066-0637* | *Website:* https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030114

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465877

DOI Link:
https://doi.org/10.5281/zenodo.19465877

Volume: 3

Issue: 1(I)

Pp. 65-68

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 12 Jan. 2026

Revised: 22 Jan. 2026

Accepted: 04 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Venkateswarlu, R. (2026). Nano material Synthesis and Characterization for Catalytic and Renewable Energy Applications. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 65–68. https://doi.org/10.5281/zenodo.19465877

Nano material Synthesis and Characterization for Catalytic and Renewable Energy Applications

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Abstract

This study investigates the synthesis and comprehensive characterization of nano materials designed for catalytic and renewable energy applications, emphasizing their critical role in advancing sustainable technologies. Employing diverse synthesis approaches including physical, chemical, and environmentally friendly green methods, the research focuses on tailoring nano material size, morphology, and surface chemistry to optimize catalytic performance.

Characterization techniques such as Transmission Electron Microscopy (TEM), X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), and X-ray Absorption Spectroscopy (XAS) were utilized to elucidate structural, compositional, and surface properties crucial for catalytic efficiency. The findings reveal that nano materials with controlled nanostructures exhibit enhanced catalytic activity, stability, and selectivity in reactions relevant to hydrogen production, CO_2 reduction, and solar energy conversion. The integration of structural insights and catalytic data underscores the relationship between material properties and performance, highlighting strategies for improving catalyst design. This research addresses challenges in scalable synthesis and mechanistic understanding, providing pathways for the development of multifunctional nano catalysts incorporating hetero structures and doping modifications.

This multidisciplinary approach leverages materials science, chemistry, and physics to deliver innovative nano materials that contribute to cleaner energy solutions and more efficient catalytic processes. The study advances the field by offering systematic methodologies for nano material development and providing a foundation for future research aimed at overcoming current limitations in renewable energy catalysis.

Keywords*: Nano materials, Catalysis, Renewable Energy, TEM, FTIR, XAS.*

Introduction

The transition to low-carbon energy systems requires catalysts with enhanced activity, selectivity, and stability that ideally rely on earth-abundant, cost-effective elements. Nano materials address these demands by providing exceptionally high surface area, a large density of exposed active sites, and tunable electronic structures owing to their nano scale dimensions and quantum confinement effects. These unique properties enable them to drive key catalytic reactions fundamental to sustainable energy, including hydrogen evolution (HER), oxygen evolution (OER), oxygen reduction (ORR), carbon dioxide reduction (CO_2RR), and biomass conversion. As a result, nano materials have emerged as transformative catalysts with the potential to significantly improve energy conversion efficiency and reduce environmental impacts.

Currently, research in nano catalysis is advancing rapidly across diverse areas such as fine chemical synthesis, hydrocarbon processing, and renewable energy systems. However, despite these advances, major challenges persist. There remain significant gaps in the mechanistic understanding of how nano structured catalysts facilitate reactions at the atomic and molecular levels, which hinders the rational design of more effective catalytic systems. Additionally, scaling laboratory synthesis methods to industrial production while maintaining nano material quality, uniformity, and performance presents formidable technical barriers.

Given these challenges, a systematic and multidisciplinary approach to nano material synthesis and characterization is essential to rational catalyst design and optimization. Controlled synthesis methods from physical and chemical routes to increasingly popular green and biogenic approaches allow precise control of particle size, shape, composition, and surface chemistry. Meanwhile, advanced characterization techniques such as high-resolution electron microscopy, X-ray absorption spectroscopy, and in situ operando spectroscopies provide critical insights into morphology, elemental composition, electronic structure, and catalyst transformations under working conditions.

Understanding the intricate correlations between nano material synthesis parameters, structural and electronic properties, and catalytic performance enables targeted modifications that enhance activity, selectivity, and stability.

Such knowledge supports the development of earth-abundant, cost-effective nano catalysts capable of replacing scarce noble metals in energy applications. In particular, advancements in doping, hetero structuring, and hierarchical nano architectures offer promising pathways for optimizing catalysts for water splitting, CO_2 reduction, solar fuel generation, and biomass upgrading. In summary, the future of low-carbon energy technologies depends heavily on the continued innovation and comprehensive study of nano material catalysts. Bridging synthesis, characterization, and application through interdisciplinary research will accelerate the design of efficient, sustainable catalytic systems necessary for a clean energy transition.

Synthesis of Nano materials:

Nano material synthesis represents a cornerstone in developing advanced catalysts for renewable energy applications, where precise control over size, shape, composition, and surface properties directly influences catalytic performance. Broadly categorized into physical, chemical, and green methods, these approaches offer complementary advantages and trade-offs in scalability, purity, and environmental impact. Physical methods prioritize high purity, chemical routes excel in tunability, and green synthesis emphasizes sustainability. This section elucidates each category, highlighting mechanisms, key parameters, representative examples, and their relevance to catalytic processes such as hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and CO_2 reduction.

1. **Physical methods**

Physical routes such as ball milling, physical vapor deposition, sputtering, and laser ablation can produce nano materials without additional chemical reducing agents. These methods are attractive for generating relatively pure metallic or oxide nano particles and thin films, often used in electro catalysis and photo catalysis. However, they can require high energy input and offer limited control over surface functionalization, so they are often combined with post-treatments or chemical modification.

2. **Chemical methods**

Chemical synthesis provides fine control over particle size, morphology, and composition. Solution-phase reduction, sol–gel processes, hydrothermal and solvo thermal methods, and chemical vapor deposition are widely used to produce metallic nano particles, metal oxides, sulfides, and carbon-based nano materials. For example, transition-metal oxides and spinels produced by hydrothermal or sol–gel routes have been optimized as catalysts and electrode materials in water electrolysis, batteries, and super capacitors. Ligands, surfactants, and reaction parameters (pH, temperature, precursor ratio) allow tailoring of nucleation and growth, directly influencing catalytic performance.

3. **Green and Sustainable Synthesis**

Rising environmental concerns and circular economy principles have propelled green synthesis, leveraging natural extracts, microbes, and enzymes as benign reductants and capping agents. These room-temperature processes minimize waste and energy use, aligning with UN Sustainable Development Goals.

Plant-mediated synthesis exploits polyphenols, flavonoids, and alkaloids in leaf extracts (e.g., neem, aloe vera) to reduce metal ions extracellularly. Gold nano particles from turmeric extract (curcumin-mediated) show plasmonic enhancement in photo catalytic H_2 production, rivaling synthetic counterparts. Fungal and bacterial routes employ extracellular enzymes (e.g., nitrate reductase in Fusarium oxysporum) for intracellular reduction, yielding Pd or Ag nano particles (5-30 nm) with protein coronas that confer biocompatibility and stability.

Advantages include one-pot synthesis avoiding harsh chemicals, scalability via bioreactor integration, and inherent functionalization for selective catalysis (e.g., biogenic Ag for 4-nitrophenol reduction). Recent advances demonstrate biogenic NiFe LDH nano sheets for OER with 300 mV overpotential, comparable to RuO_2. Challenges encompass polydispersity (20-50% variation), batch inconsistencies from biological variability, and lower yields (<50%). Standardization via optimized extraction protocols and genetic engineering of microbes addresses these. Hybrid green-chemical cascades, combining extracts with hydrothermal aging, enhance crystallinity.

Integrating green synthesis with life-cycle assessments promises carbon-neutral nano catalyst production, with downstream recycling via magnetic separation amplifying sustainability. In summary, selecting synthesis routes hinges on application demands: physical for purity, chemical for precision, and green for eco-compatibility. Hybrid methodologies will likely prevail, enabling multifunctional nano materials for next-generation renewable energy catalysis.

Characterization Techniques:

Comprehensive characterization bridges nano material synthesis with catalytic performance, establishing structure-property-performance relationships essential for rational design in renewable energy applications. Multi-modal techniques spanning microscopy, spectroscopy, diffraction, and electrochemistry provide atomic-scale insights into morphology, composition, electronic structure, and dynamic behavior under operating conditions. This section details key methods across structural, surface, and functional domains, emphasizing their synergies and operando capabilities for advancing nano catalysts in HER, OER, CO_2RR, and photo catalysis.

1. **Structural and morphological characterization**

High-resolution imaging and diffraction techniques are essential to establish structure–property correlations. Transmission electron microscopy (TEM) and high-resolution TEM reveal particle size distribution, shape, and lattice fringes, while scanning electron microscopy (SEM) is used to probe surface morphology and aggregation. X-ray diffraction (XRD) provides information on crystallinity, phase composition, and average crystallite size. For complex nanostructures such as core–shell or hetero structured catalysts, electron tomography and small-angle scattering are increasingly used to resolve three-dimensional architectures.

2. **Surface and chemical analysis**

The catalytic performance of nano materials is strongly governed by surface composition, oxidation state, and defect chemistry. X-ray photoelectron spectroscopy (XPS), X-ray absorption spectroscopy (XAS), including XANES and EXAFS, and Energy-Dispersive X-ray spectroscopy (EDX) are routinely applied to probe surface and near-surface chemistry. Infrared and Raman spectroscopy provide insight into functional groups, adsorbates, and reaction intermediates, while Brunauer–Emmett–Teller (BET) analysis quantifies surface area and porosity, both crucial for heterogeneous catalysis and electrochemical processes.

3. **Physical and electrochemical properties**

For energy applications, it is vital to measure electronic, optical, and electrochemical properties. UV-Vis and photoluminescence spectroscopy probe band-gap and light-harvesting capabilities relevant to photo catalysts and photo electrodes. Electrochemical methods-cyclic voltammetry, linear sweep voltammetry, impedance spectroscopy, and chronoamperometry-quantify overpotential, Tafel slopes, charge-transfer resistance, and stability of electro catalysts for key reactions such as HER, OER, ORR, and CO_2RR. Thermal analysis (TGA/DSC) and mechanical testing, where relevant, further inform stability and integration into devices.

Nano materials in catalytic renewable energy reactions:

Nano materials revolutionize catalytic processes for renewable energy by maximizing active site exposure, tuning electronic properties, and facilitating charge/mass transport in key reactions driving the hydrogen economy, carbon utilization, and sustainable fuels.

1. **Water splitting and hydrogen production**

Hydrogen evolution and oxygen evolution are central to electrochemical and photo electrochemical water splitting. Noble-metal catalysts, especially Pt for HER and Ir/Ru oxides for OER, set performance benchmarks but suffer from high cost and scarcity. Recent research focuses on nano structured transition-metal sulfides, phosphides, carbides, and doped oxides as cost-effective alternatives. Nano structuring enhances surface area and exposes active edge sites, while doping and hetero structuring modulates electronic structure to lower overpotential and improve stability.

2. **CO_2 reduction and fuel production**

Electrochemical and photo catalytic CO_2 reduction convert waste CO_2 into value-added fuels and chemicals. Nano structured copper, silver, and molecularly modified carbon materials have been explored to steer selectivity toward CO, formate, hydrocarbons, or alcohols. Controlling surface defects, grain boundaries, and local coordination environments in nano materials is key to tuning binding energies of intermediates and suppressing competing hydrogen evolution. Coupling CO_2 reduction catalysts with light-harvesting semiconductors or tandem cell architectures is an active area of materials research.

3. **Solar-driven and biomass-based catalysis**

Semiconductor nano materials such as TiO_2, perovskites, and complex oxides, often combined with plasmonic or co-catalyst nano particles enable photo catalytic water splitting, pollutant degradation, and solar-fuel generation. For biomass conversion, nano structured zeolites, metal-supported catalysts, and enzymatic hybrids improve efficiency and selectivity in transforming lingo cellulosic feedstocks into bio fuels and platform chemicals. In both cases, optimizing interfaces between phases metal/oxide, catalyst/support, or enzyme/inorganic requires careful structural and surface characterization.

Structure–property–performance relationships:

A central theme in current literature is the quantitative linking of nanostructure and composition to catalytic metrics such as activity, selectivity, and durability. Studies on complex nano materials show that parameters including particle size, shape, exposed facets, defect density, and hetero junction design collectively determine performance in energy-relevant reactions. Advanced in situ and operando techniques are increasingly employed to monitor phase changes, oxidation-state dynamics, and adsorbate evolution under reaction conditions, providing mechanistic insight not accessible from ex situ measurements alone.

Challenges and future directions:

Despite rapid progress, several challenges hinder the deployment of nano material-based catalysts in large-scale energy systems. These include:

- Scalability and reproducibility of synthesis while maintaining precise control over nano scale features.
- Long-term stability under realistic operating conditions, including corrosion, sintering, and poisoning.
- Comprehensive mechanistic understanding across time and length scales, requiring integration of experiments with multi scale modeling and machine-learning-guided screening.
- Environmental and health considerations related to nano particle synthesis, use, and end-of-life management, motivating greener synthesis and safer-by-design strategies.

Future research is likely to focus on complex, multifunctional nano materials such as core-shell structures, high-entropy alloys, and hierarchical porous frameworks—that can simultaneously optimize activity, selectivity, and robustness. Combining green synthesis routes with data-driven design and operando characterization will be critical for translating laboratory-scale advances into industrially relevant catalytic technologies.

Conclusion:

Nano materials have transformed the landscape of catalysis and renewable energy research by enabling precise control over active sites, reaction pathways, and local reaction environments. Their high surface-to-volume

ratio, tunable composition, and engineered nano-architectures allow optimization of key performance metrics such as activity, selectivity, and durability across reactions including HER, OER, ORR, CO_2 reduction, and biomass conversion. A clear understanding of how synthesis routes dictate crystallinity, morphology, defect density, and surface chemistry and how these structural features are revealed by advanced characterization is indispensable for rational catalyst design rather than empirical trial-and-error.

Equally crucial is the integration of operando and in situ characterization with theoretical modeling and data-driven approaches to uncover structure–property–performance relationships under realistic operating conditions. This knowledge base will guide the development of robust, earth-abundant, and scalable nano catalysts tailored for specific energy conversion and storage technologies. Continued progress will depend on strongly interdisciplinary efforts that link materials science, physics, chemistry, and engineering, and increasingly incorporate machine learning, process intensification, and life-cycle assessment. Such coordinated strategies are essential to translate laboratory-scale nano material innovations into practical devices and systems that contribute meaningfully to global clean energy and environmental sustainability targets.

Acknowledgements:
The author thanks the principal and faculty of the Department of Physics, Government Degree College (A), Khairatabad, Hyderabad, and the Principal, Government Degree College (A), Nalgonda.

Financial support and sponsorship
Nil.

Conflicts of interest
The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030115

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465917

DOI Link:
https://doi.org/10.5281/zenodo.19465917

Volume: 3

Issue: 1(I)

Pp. 69-74

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 12 Jan. 2026

Revised: 22 Jan. 2026

Accepted: 04 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Kantankar, A., & M. Sunitha. (2026). Assessment of Composition of Selected Heavy Metals in Road Dust from Sangareddy Region. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 69–74.
https://doi.org/10.5281/zenodo.19465917

Assessment of Composition of Selected Heavy Metals in Road Dust from Sangareddy Region

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Abstract

Road dust is recognized as a significant reservoir of heavy metals originating from vehicular emissions, industrial activities, and urban development. This study focuses on the assessment of the composition and concentration of selected heavy metals in road dust collected from the Sangareddy region. Representative samples were systematically collected from high-traffic, commercial, and residential areas to evaluate spatial variations in contamination levels. The collected samples were processed and analyzed using standard analytical techniques to determine the concentrations of heavy metals such as lead (Pb), cadmium (Cd), chromium (Cr), nickel (Ni), zinc (Zn), and copper (Cu). The results revealed considerable variation in metal concentrations across different locations, with higher levels observed in areas experiencing dense traffic and industrial influence. Comparative analysis with permissible limits indicated that certain metals exceeded recommended thresholds, suggesting potential environmental and health risks.

Statistical analysis and contamination indices were employed to identify possible sources and the degree of pollution. The findings indicate that vehicular emissions, wear and tear of automobile components, and anthropogenic activities are the primary contributors to heavy metal accumulation in road dust. This study highlights the need for regular monitoring and effective pollution control strategies to mitigate heavy metal contamination in urban environments, thereby reducing associated ecological and human health risks.

Keywords: *Road dust, Heavy metals, Sangareddy region, Environmental pollution, Urban contamination, Vehicular emissions, Toxic elements, Pollution assessment*

Introduction

Urban environments worldwide are undergoing rapid structural and functional changes due to accelerated urbanization and shifting socio-economic conditions [1–2]. This growth has intensified industrial activity and vehicular density, which are major drivers of urban air pollution. Consequently, urban surfaces increasingly act as sinks for atmospheric fallout from multiple sources, particularly local anthropogenic inputs [3]. Motor vehicles contribute significantly through exhaust emissions, brake and tire wear, and mechanical abrasion, leading to heavy contamination of road dust [4]. Road dust is a heterogeneous matrix formed by complex interactions of solid, liquid, and gaseous pollutants derived mainly from traffic-related emissions and other urban activities [5–6]. Its generation and chemical composition depend on climatic conditions, traffic intensity, land-use patterns, and regional geology [7]. Several studies report that road dust is enriched with heavy metals and organic contaminants [8–9]. Heavy metals accumulate through sedimentation and deposition processes, with inputs from industrial emissions, lubricant leakage, fuel combustion, and corrosion of vehicle parts and infrastructure [10]. The ecological and health risks depend on metal concentration, speciation, bioavailability, and mobility [11]. Heavy metal contamination of roadside soils and vegetation has gained global attention due to increasing highway traffic and industrial corridor expansion [12–13]. Roadside soils often show elevated metal loads, especially near industrial belts or mining regions, and coal-derived particulates can further enrich soils with trace metals [14]. Major sources include road surface degradation, combustion emissions, oil leakage, brake/tire wear, mining, metallurgical processing, battery corrosion, thermal power emissions, pesticide use, and weathering of metallic materials [15–16]. Persistent metals such as Cd, Cr, Cu, Pb, Zn, and Ni may cause long-term ecological degradation and health risks through inhalation, dermal contact, and ingestion pathways [17–18]. Road-deposited sediments accumulate heavy metals above background levels and may be resuspended during dry seasons or mobilized through runoff, contaminating soils and waters [19]. Numerous studies have documented elevated concentrations of heavy metals in urban and roadside environments [20–22]. Within India, investigations of Sangareddy's urban soils have revealed contamination levels associated with both carcinogenic and non carcinogenic risks.

Building on this evidence, the present study examines Pb, Zn, Cd, Fe, Mn, and Ni in road dust from Sangareddy to evaluate their spatial distribution and contamination status.

Study Area:

Established in 1954, Sangareddy Municipality is classified as a first-grade municipality with 38 electoral wards. It administers an area of 13.69 km², while the city's overall urban expansion has increased to nearly 45 km² due to rapid growth and infrastructure development [23]. In recent years, Sangareddy district has evolved into a major industrial corridor, attracting several national and regional enterprises **[24]**. Key industrial sectors include pharmaceuticals and biotechnology (Sangareddy Pharma SEZ with firms such as Dr. Reddy's Laboratories and Hetero Drugs), chemicals and petrochemicals (specialty chemicals, polymers, and industrial intermediates), textiles and garments (Textile Park with spinning, weaving, and garment units), agro-processing (food processing and dairy-based industries), automobile and engineering (component and machinery manufacturing including Bharat Forge), renewable energy (solar park and wind energy projects), and construction and real estate driven by sustained urbanization.

Methodology:

Inductively coupled plasma–mass spectrometry (ICP–MS) is a highly sensitive technique used for trace and ultra-trace elemental analysis in environmental and biological samples. Compared with AAS and AES, it provides lower detection limits, rapid multi-element capability, and high analytical throughput. Reliable analysis requires proper understanding of instrument operation and careful control of spectroscopic (polyatomic/isobaric) and non-spectroscopic (matrix) interferences.

A typical single-quadrupole ICP–MS consists of a sample introduction system (nebulizer and spray chamber), an argon plasma source, interface cones (sampler and skimmer), ion optics, a quadrupole mass analyzer, and a detector. Liquid samples are nebulized into an aerosol and introduced into the plasma, where desolvation, atomization, and ionization occur. The ions are extracted through the interface, focused by electrostatic lenses, separated according to mass-to-charge ratio (m/z), and detected for quantification.

The ICP source operates at ~6000–10,000 K and is sustained in argon using RF energy applied through a load coil surrounding a quartz torch. Argon carrier, auxiliary, and coolant gases ensure efficient transport, discharge stability, and torch protection.

Materials And Methods

Sampling sites:

Road dust was collected from Sangareddy region from various geographical areas including Industrial, Residential, and Eco-conservative zonesDust samples were gathered from the pavements located on both sides of the roads at the designated sampling points. After collection, each sample was placed in borosilicate bottles, properly labeled, and subsequently transported to the laboratory for analysis.

Sample Digestion and Heavy Metal Determination:

Approximately 1 g of each road dust sample was subjected to acid digestion using 16 mL of concentrated nitric acid (HNO_3) and 4 mL of perchloric acid ($HClO_4$). The mixture was heated on a hot plate at 85 °C for one hour. The resulting solution was passed through a 0.45 µm Whatman glass microfiber filter (47 mm) under vacuum. The filtrate was then diluted to a final volume of 100 mL with deionized water and preserved in polyethylene bottles at 4 °C until further analysis.

Quantification of heavy metals (Pb, Cd, Cu, Zn, Fe, Mn, Ni) was performed using inductively coupled plasma–mass spectrometry (ICP–MS, PerkinElmer ELAN 9000). Calibration standards were prepared by serial dilution of certified 1000 mg/L stock solutions. Method validation indicated recoveries ranging from 69% to 120%, confirming acceptable analytical accuracy. Elevated concentrations of metals were observed in samples collected from industrial zones compared to other areas.

Results And Discussions:

Analysis of roadside dust across Sangareddy revealed pronounced spatial heterogeneity, reflecting distinct pollution gradients within the region. Elevated concentrations of Pb, Cu, Zn, Fe, and Mn were detected at Patancheru and Isnapur, whereas comparatively lower levels were observed at Tara Government College, Sangareddy Bus Stand, and the Manjeera Reservoir area. These findings highlight the influence of localized industrial activity on the distribution of heavy metals in urban dust. This enrichment is mainly attributed to intense industrial activity and rapid urban development in these areas. Elevated concentrations of toxic metals, particularly Pb, Cd, and Ni, pose serious public health concerns due to their persistence and bioaccumulative nature. Human exposure occurs primarily through inhalation of resuspended dust and accidental ingestion, potentially causing neurotoxicity, respiratory disorders, renal damage, and carcinogenic effects. Environmentally, metal deposition contaminates soils and surface waters, disrupts ecosystem functioning, and reduces biodiversity.

Industrial emissions, metallurgical operations, waste disposal, and fuel combustion are probable sources in Patancheru and Isnapur, while traffic-related inputs contribute significantly near high-traffic zones such as Sangareddy Bus Stand. In some locations, metal concentrations exceeded guideline limits, highlighting contamination hotspots and the need for immediate mitigation. Future work should focus on particle-size distribution, bioavailability, and long-term risk assessment.

Table 1: Heavy metal content in Dust sample collected from various locations of Sangareddy.

Sample	Sampling Site	Geo-location	Pb	Cd	Cu	Zn	Fe	Mn	Ni
Sample-1	Patancheru	17.53°N 78.27°E.	247.89	1.17	237.11	560.89	17750.87	390.11	51.78
Sample-2	Isnapur	17°32′55″N 78°12′37″E.	201.7	1.01	219.88	589.01	17007.9	317.1	47.01
Sample-3	Tara Government College (A), Sangareddy	17.606525 N, 78.076422 E.	112.32	0.19	178.11	499.17	9007.88	270.12	40.1
Sample-4	Sangareddy Bus stand	17.6152047 N, 78.0816250E.	170.12	0.31	156.71	510.13	12009.1	310.18	39.78
Sample-5	Manzeera Reservoir	17.661859 N, 78.079561 E.	95.1	0.09	127.89	489.1	8901.89	234.57	37.89

All the values are expressed in ppm.

Research Findings:

Patancheru: An industrial area exhibiting the highest concentrations of most metals, including lead (Pb: 247.89 ppm), copper (Cu: 237.11 ppm), zinc (Zn: 560.89 ppm), and iron (Fe: 17750.87 ppm).

Isnapur: Another industrialized region with elevated levels of Pb (201.7 ppm), Cu (219.88 ppm), Zn (589.01 ppm), and Fe (17007.9 ppm), though slightly lower than Patancheru.

Tara Government College and Manjeera Reservoir: These areas, farther from industrial zones, had considerably lower concentrations of all measured metals:

Tara College: Pb (112.32 ppm), Cu (178.11 ppm), Zn (499.17 ppm), Fe (9007.88 ppm).

Manjeera Reservoir: Pb (95.1 ppm), Cu (127.89 ppm), Zn (489.1 ppm), Fe (8901.89 ppm).

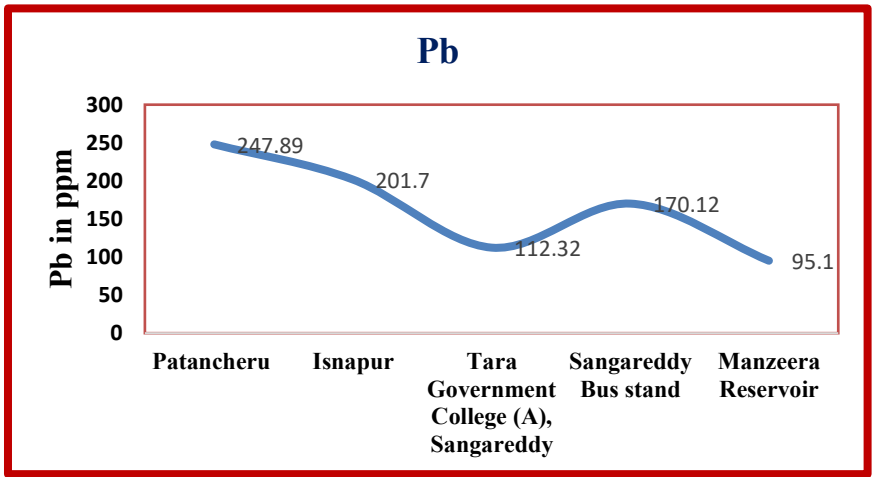


Figure 1: Lead content in dust samples.

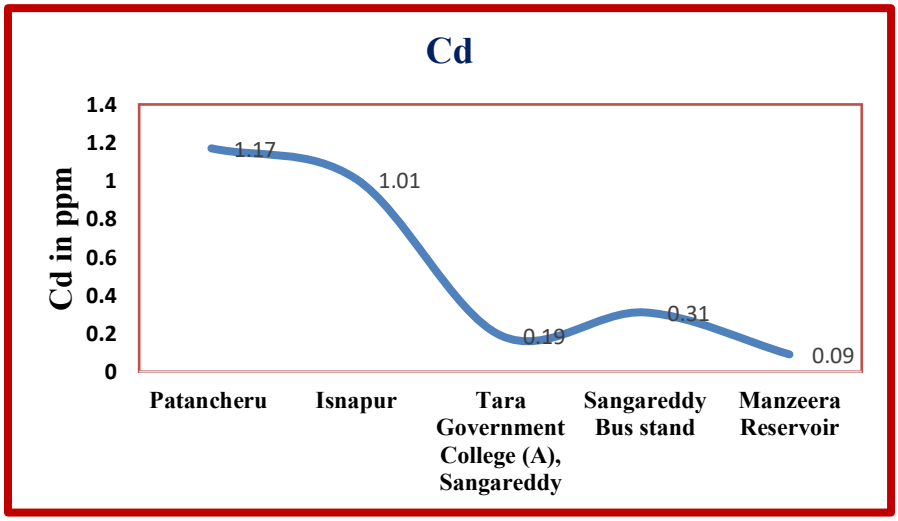


Figure 2: Cadmium content in dust samples.

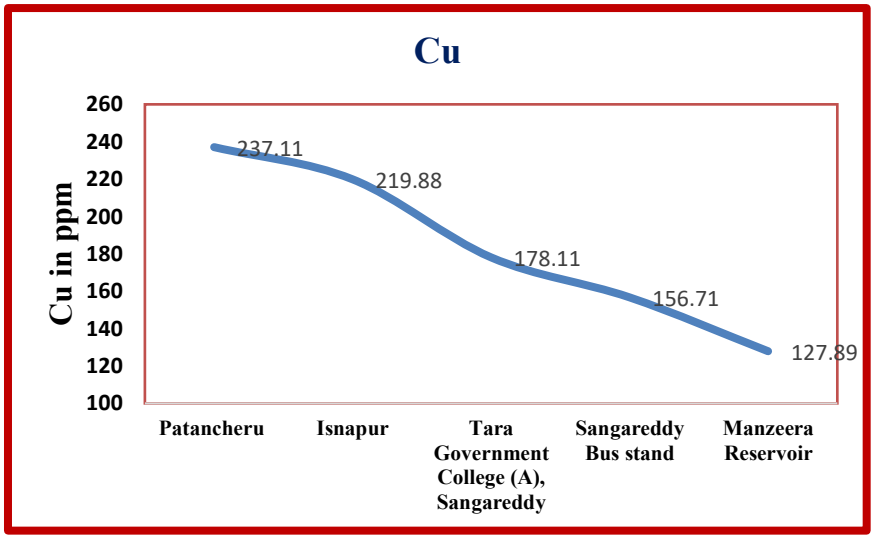


Figure 3: Copper content in dust samples.



Figure 4: Zinc content in dust samples.

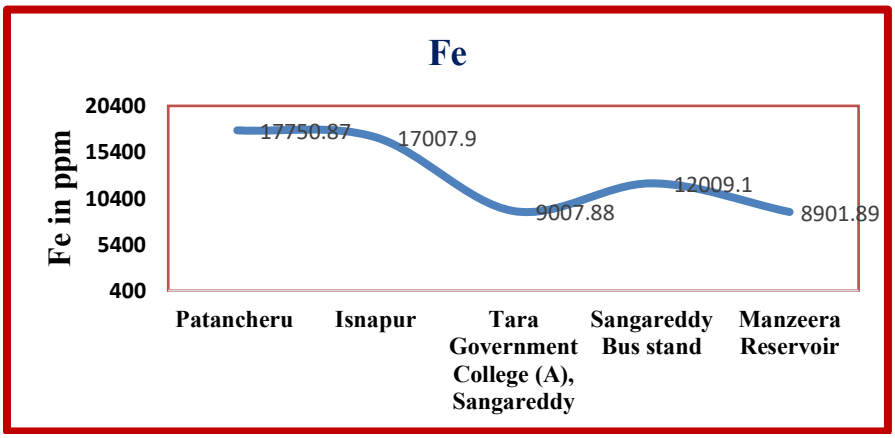


Figure 5: Iron content in dust samples.

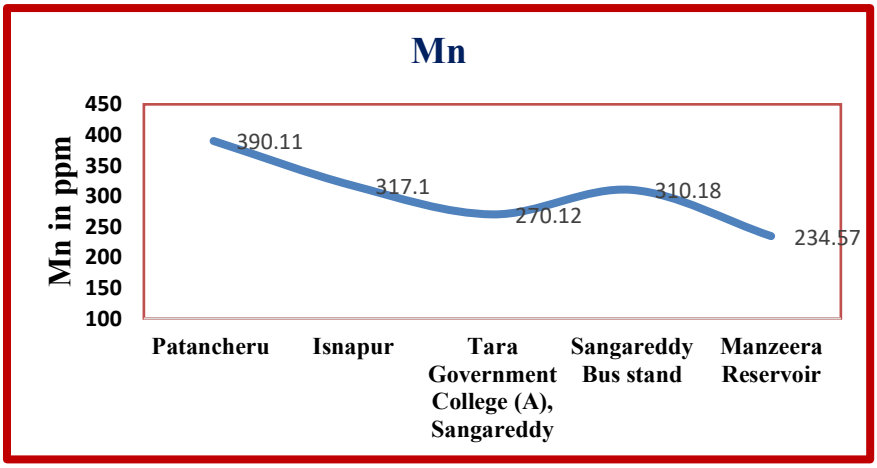


Figure 6: Manganese content in dust samples.

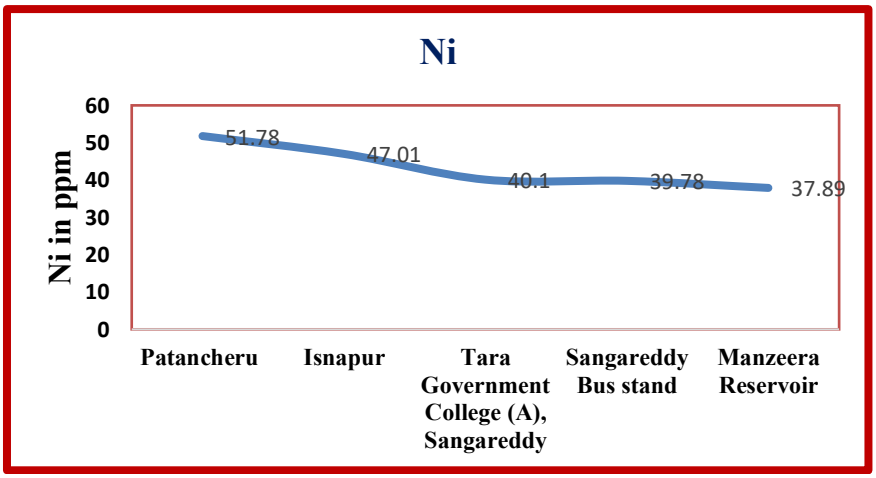


Figure 7: Nickel content in dust samples.

Conclusion:

The roadside dust assessment in Sangareddy demonstrated marked spatial variability in heavy metal loading, with industrial zones such as Patancheru and Isnapur exhibiting the highest enrichment, likely driven by industrial emissions and metal-processing activities. The elevated metal concentrations indicate potential human health risks and highlight the need for further evaluation of particle-size distribution, metal bioavailability, and chronic exposure pathways. Implementation of effective mitigation and pollution control measures is essential to minimize contamination and safeguard public health.

Acknowledgment

I would like to express my sincere gratitude to all those who supported and contributed to the successful completion of this study on Assessment of Composition of Selected Heavy Metals in Road Dust from Sangareddy Region.

I am deeply thankful to my guide/supervisor for their constant encouragement, valuable guidance, and constructive suggestions throughout the course of this research. Their expertise and support were instrumental in the completion of this work.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030116

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19465974

DOI Link:
https://doi.org/10.5281/zenodo.19465974

Volume: 3

Issue: 1(I)

Pp. 75-78

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 12 Jan. 2026

Revised: 22 Jan. 2026

Accepted: 04 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
V. Sahiti, & P. Pushpalatha. (2026). Microplastics and Nanoplastics in the Environment: Chemical and Biochemical Strategies for Effective Degradation. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 75–78.
https://doi.org/10.5281/zenodo.19465974

Microplastics and Nanoplastics in the Environment: Chemical and Biochemical Strategies for Effective Degradation

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Abstract

Microplastics (<5 mm) and nanoplastics (<1 μm) are persistent environmental pollutants formed from fragmentation of synthetic polymers. Their small size, high surface area, and resistance to natural breakdown allow accumulation across ecosystems and potential transfer of contaminants, raising ecological and human health concerns. Conventional waste management fails to address diffuse particles, driving research toward advanced degradation methods. This review evaluates chemical (photodegradation, pyrolysis, advanced oxidation), biochemical (enzymatic, microbial), and hybrid strategies. Chemical methods achieve rapid chain scission but often produce secondary pollutants and incomplete mineralization. Biochemical approaches offer specificity and potential full mineralization, though limited by crystallinity and kinetics. Hybrid systems combining oxidative pretreatment with enzymatic/microbial degradation show the highest promise. Emerging tools (enzyme engineering, AI, computational modeling) and environmental safety considerations are discussed. Scalability, cost, field validation, and standardized analytics remain major challenges.

Keywords: *Microplastics, Nanoplastics, PETase, Microbial consortia, advanced oxidation, Hybrid degradation*

Introduction

Annual global plastic production exceeds 400 million tons, with mismanaged waste fragmenting into microplastics (MPs) and nanoplastics (NPs) that pervade marine, freshwater, terrestrial, and atmospheric compartments (Geyer et al., 2017; Andrady, 2011). These particles adsorb pollutants and form biofilms, acting as vectors in food webs and appearing in human tissues (Leslie et al., 2022). Polyolefins (PE, PP) resist degradation due to stable C–C backbones and high crystallinity, while polyesters (PET) contain more susceptible ester bonds (Tokiwa et al., 2009; Wei & Zimmermann, 2017). Conventional recycling and incineration are inadequate for diffuse contamination, motivating development of targeted chemical and biochemical degradation technologies.

Physicochemical Properties Influencing Degradation

Degradation susceptibility depends on:

- **Backbone chemistry** — C–C bonds (polyolefins) resist hydrolysis; ester bonds (PET) are enzymatically cleavable.
- **Crystallinity** — >35–40% reduces enzyme and oxidant access; amorphous regions degrade faster.
- **Surface chemistry** — Hydrophobicity limits water/enzyme contact; oxidation introduces polar groups (carbonyl index ↑).
- **Particle size** — NPs show higher surface reactivity, adsorption, and bioavailability.
- **Additives** — Stabilizers slow degradation; leaching increases porosity but adds secondary pollutants. Environmental weathering usually causes fragmentation rather than mineralization, increasing NP abundance (Gigault et al., 2018).

Table 1. Key physicochemical determinants

Polymer	Dominant Mechanism	Relative Persistence	Main Limitation
PE	Oxidative chain scission	Very high	Hydrophobicity
PP	Photo-oxidation	Very high	Tertiary C stability
PET	Ester hydrolysis	High	Crystallinity
PS	Radical oxidation	High	Steric hindrance

Chemical Degradation Approaches

Chemical degradation methods induce rapid structural modifications in plastics but rarely achieve complete mineralization to CO_2 and H_2O (Rahimi & García, 2017; Mohanan et al., 2020).

Photodegradation

Ultraviolet (UV) radiation initiates free-radical oxidation reactions in polymer chains, resulting in chain scission, carbonyl formation, surface embrittlement, and fragmentation into micro- and nanoplastics (Andrady, 2011; Barnes et al., 2009). However, the process is slow under natural environmental conditions due to limited UV intensity and oxygen availability.

Pyrolysis and catalytic pyrolysis

Thermal degradation at elevated temperatures (300–800 °C) converts polymers into fuels, oils, and char through random chain cleavage and depolymerization (Rahimi & García, 2017). Catalytic pyrolysis improves product selectivity and lowers energy requirements but remains energy-intensive and more suitable for bulk plastic waste rather than dispersed microplastics.

Advanced Oxidation Processes (AOPs)

Hydroxyl radicals (•OH) generated through Fenton reactions, photocatalysis using TiO_2 or ZnO, or UV/H_2O_2 systems rapidly oxidize polymer surfaces, increasing oxygen-containing functional groups such as carbonyl and hydroxyl groups (Mohanan et al., 2020). While effective for surface activation, challenges include incomplete mineralization, catalyst recovery, and potential formation of secondary oxidation by-products. Overall, chemical methods are particularly effective as pretreatment strategies, increasing hydrophilicity, surface roughness, and reducing crystallinity, thereby improving susceptibility to subsequent enzymatic and microbial degradation (Wei & Zimmermann, 2017).

Biochemical and Microbial Degradation

Biochemical degradation offers greater specificity and operates under environmentally compatible conditions, enabling controlled polymer depolymerization and potential mineralization (Urbanek et al., 2018).

Enzymatic hydrolysis

Specific enzymes such as PETase and MHETase from *Ideonella sakaiensis* catalyze the hydrolysis of PET into terephthalic acid (TPA) and ethylene glycol (EG), enabling complete polymer depolymerization (Yoshida et al., 2016). Engineered PET hydrolases have demonstrated significantly enhanced activity and thermostability, improving degradation efficiency under industrial conditions (Tournier et al., 2020; Lu et al., 2022). Additionally, cutinases, lipases, laccases, and peroxidases contribute to degradation of polyesters and oxidized polyolefins (Wei & Zimmermann, 2017; Carniel et al., 2021).

Microbial assimilation

Various bacterial genera, including *Pseudomonas* and *Rhodococcus*, and fungal species such as Phanerochaete chrysosporium and Aspergillus niger, oxidize polymer surfaces and metabolize degradation intermediates through central metabolic pathways such as the β-ketoadipate pathway and the tricarboxylic acid (TCA) cycle (Urbanek et al., 2018). Microbial colonization of plastics, known as the "plastisphere," facilitates biodegradation through extracellular enzyme secretion (Zettler et al., 2013).

Microbial consortia

Mixed microbial communities exhibit synergistic degradation capabilities, combining oxidative, hydrolytic, and assimilatory functions. Fungal species often initiate oxidative modification, followed by bacterial assimilation and mineralization, resulting in greater degradation efficiency compared to monocultures (Urbanek et al., 2018).
Despite these advantages, biochemical degradation remains limited by slow kinetics, restricted enzyme accessibility in highly crystalline polymers, and inherent resistance of polyolefins due to stable C–C backbone structures (Wei & Zimmermann, 2017).

Hybrid Chemical–Biochemical Strategies

Hybrid approaches combining chemical pretreatment with biological degradation represent the most effective and practical strategy for plastic remediation (Mohanan et al., 2020).

Pretreatment enhances biodegradability

Oxidative treatments such as UV irradiation, Fenton oxidation, plasma exposure, and photocatalysis introduce oxygen-containing functional groups, increase surface roughness, and reduce crystallinity, thereby improving enzyme accessibility and microbial colonization (Wei & Zimmermann, 2017).

Sequential degradation pathways

Hybrid systems typically follow a stepwise process involving initial oxidation to weaken polymer structure, enzymatic hydrolysis to depolymerize polymer chains, and microbial metabolism to achieve mineralization (Urbanek et al., 2018).

Integrated photocatalytic–biological systems

Photocatalytic pretreatment combined with bioreactor-based enzymatic or microbial degradation has demonstrated improved degradation efficiency and scalability potential (Mohanan et al., 2020).

AI-assisted enzyme engineering

Recent advances in machine learning and computational modeling have accelerated the discovery and optimization of plastic-degrading enzymes, significantly improving catalytic efficiency, stability, and substrate specificity (Lu et al., 2022).

These hybrid strategies overcome individual limitations of chemical and biological methods and represent the most promising approach for scalable and sustainable plastic degradation.

Environmental Safety and Toxicity Considerations

Incomplete plastic degradation can generate toxic intermediates, oxidized oligomers, and smaller nanoplastic particles that may exhibit increased bioavailability and biological reactivity (Gigault et al., 2018; Chae & An, 2017). Nanoplastics can cross biological membranes, accumulate in tissues, and induce oxidative stress, inflammation, and cellular dysfunction, raising concerns for ecological and human health (Mattsson et al., 2015; Wright & Kelly, 2017). Therefore, complete mineralization into CO_2, H_2O, and microbial biomass represents the safest and most environmentally desirable endpoint (Mohanan et al., 2020).

Hybrid degradation systems that emphasize biological mineralization following controlled oxidative pretreatment reduce the accumulation of harmful intermediates compared to purely chemical processes (Wei & Zimmermann, 2017; Urbanek et al., 2018). Additionally, ecotoxicological evaluation of degradation products using standardized bioassays and long-term environmental monitoring is essential to ensure ecological safety and regulatory compliance (Rochman et al., 2013; Mohanan et al., 2020).

Roadmap to Scalability and Life-Cycle Assessment (LCA)

The translation of plastic degradation technologies from laboratory-scale experiments to industrial-scale implementation requires a systematic roadmap that integrates technical efficiency, economic feasibility, and environmental sustainability (Rahimi & García, 2017).

1. Balancing Energy and Environmental Benefit

A critical factor in evaluating degradation technologies is the net environmental benefit. High-energy processes such as pyrolysis and UV-intensive advanced oxidation may offset environmental gains if their energy consumption exceeds the environmental burden of the plastic waste itself (Rahimi & García, 2017; Mohanan et al., 2020).

- **Low-energy inputs** — Sustainable approaches should prioritize solar-driven photocatalysis and ambient-temperature enzymatic and microbial degradation systems, which reduce carbon emissions and improve energy efficiency (Wei & Zimmermann, 2017; Urbanek et al., 2018).
- **Catalyst circularity** — Catalyst recovery and reuse are essential to minimize operational costs and prevent secondary environmental contamination. Recyclable photocatalysts such as TiO_2 and engineered enzymes with improved stability and reusability enhance process sustainability (Mohanan et al., 2020; Lu et al., 2022).
- **By-product valorization (upcycling)** — Instead of complete mineralization alone, degradation strategies should aim to recover valuable intermediates such as monomers (e.g., terephthalic acid and ethylene glycol) or microbial biomass, contributing to circular economy models and improving economic feasibility (Rahimi & García, 2017; Tournier et al., 2020).

2. Standardized Analytics and Field Validation

The lack of standardized analytical methods currently limits comparison and validation of degradation technologies across studies (Gigault et al., 2018; Mohanan et al., 2020).

- **Quantifying mineralization** — Reliable assessment of degradation requires standardized measurement of CO_2 evolution using respirometry and advanced analytical techniques such as gas chromatography–mass spectrometry (GC-MS) and isotope tracing to confirm complete mineralization (Mohanan et al., 2020).
- **From laboratory polymers to environmental plastics** — Most studies use pristine polymers, whereas environmental plastics undergo weathering, oxidation, and biofilm formation, altering degradation behavior. Field validation must therefore incorporate environmentally aged plastics and plastisphere microbial communities (Zettler et al., 2013; Gigault et al., 2018).
- **Life-Cycle Assessment (LCA)** — Comprehensive LCA frameworks are necessary to evaluate the environmental footprint, including global warming potential, toxicity, and energy consumption, of degradation technologies compared to conventional waste management strategies such as landfilling and incineration (Rahimi & García, 2017; Mohanan et al., 2020).

Conclusion

No single degradation strategy is sufficient to address the persistence and environmental distribution of microplastics and nanoplastics. Chemical methods can rapidly alter polymer structure through oxidation and chain scission, but they rarely result in complete mineralization. In contrast, enzymatic and microbial processes provide higher substrate specificity and operate under environmentally favorable conditions, although their efficiency is often constrained by slow reaction rates and limited accessibility to highly crystalline polymers (Wei & Zimmermann, 2017; Urbanek et al., 2018).

Current evidence indicates that combined approaches, in which oxidative pretreatment enhances polymer accessibility followed by enzymatic depolymerization and microbial assimilation, offer greater degradation efficiency than individual methods alone (Mohanan et al., 2020). Such integrated systems improve enzyme access, accelerate depolymerization, and support subsequent microbial conversion of degradation products. Recent developments in

enzyme engineering and computational design have further improved catalytic performance and stability, increasing the feasibility of large-scale applications (Tournier et al., 2020; Lu et al., 2022).

In the long term, successful implementation will depend on integrating these technologies into sustainable waste management systems supported by life-cycle assessment and circular economy principles. These approaches enable not only environmental remediation but also recovery of valuable intermediates, contributing to more sustainable plastic management practices (Rahimi & García, 2017).

Acknowledgment

I would like to express my sincere gratitude to everyone who contributed to the successful completion of this work on Microplastics and Nanoplastics in the Environment: Chemical and Biochemical Strategies for Effective Degradation.

First and foremost, I am deeply thankful to my guide/supervisor for their invaluable guidance, constant encouragement, and insightful suggestions throughout the course of this study. Their expertise greatly contributed to the development and completion of this research.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| *Volume-3 Issue-1(I)* | *February-2026* | *ISSN: 3066-0637* | *Website:* https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030117

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19466009

DOI Link:
https://doi.org/10.5281/zenodo.19466009

Volume: 3

Issue: 1(I)

Pp. 79-82

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 12 Jan. 2026

Revised: 22 Jan. 2026

Accepted: 04 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
V. Saritha Rani. (2026). Green Solvents and Their Impact on Sustainable Chemical Process Design: A Review. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 79–82.
https://doi.org/10.5281/zenodo.19466009

Green Solvents and Their Impact on Sustainable Chemical Process Design: A Review

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Abstract

The increasing emphasis on environmentally responsible chemical manufacturing has significantly intensified interest in sustainable process design across both academia and industry. Solvents represent a major share of material usage in chemical processes and are often responsible for substantial waste generation, emissions and environmental burden. As a result, solvent selection has emerged as a critical decision point in improving the overall sustainability, safety, and efficiency of chemical manufacturing operations. Green solvents offer a practical and effective strategy to reduce environmental impact while maintaining or in some cases enhancing, process performance and product quality. This review critically examines the role of green solvents in the design of sustainable chemical processes, emphasizing their potential to replace conventional hazardous solvents without compromising technical feasibility.

Various classes of green solvents including bio-based solvents, ionic liquids, deep eutectic solvents, supercritical fluids and aqueous systems are systematically discussed with respect to their physicochemical properties, environmental compatibility and industrial applicability. Overall, the review highlights how green solvents play a vital role in enabling safer, cleaner, and more resource-efficient chemical processes, thereby supporting the broader goals of sustainable development in the chemical industry.

Keywords: *green solvents, sustainable process design, green chemistry, environmentally benign solvents, solvent selection.*

Introduction

The growing demand for environmentally responsible chemical manufacturing has intensified interest in sustainable process design. The choice of solvents is crucial for sustainability since they make up a significant amount of material consumption and waste production in the chemical industries. Green solvents provide a practical solution to reduce environmental impact without sacrificing process efficiency.

The function of green solvents in sustainable chemical process design is examined extensively in this paper. The physicochemical characteristics, environmental performance and industrial applicability of several types of green solvents—such as bio-based solvents, ionic liquids, deep eutectic solvents, supercritical fluids, and aqueous systems—are examined. Green solvent adoption's effects on the environment, economy and operations are examined, along with present constraints and potential future developments. The review emphasizes how green solvents help make chemical processes safer, cleaner and more resource-efficient.

In chemical synthesis, separation, purification and formulation, solvents are essential. Solvents make up the majority of the material input and waste output in many industrial processes. Because of their toxicity, volatility, flammability and environmental persistence, conventional organic solvents like benzene, toluene, dichloromethane, and N, N-dimethyl formamide present significant concerns.

The goal of sustainable chemical process design is to lessen these adverse effects while maintaining economic viability and productivity. The reduction of waste, decreased risk, energy efficiency and the utilization of renewable feed stocks are the main tenets of green chemistry. Solvent substitution is seen as one of the most effective tactics among these concepts. Green solvents offer safer substitutes that promote sustainability goals in the social, economic and environmental spheres.

The increasing emphasis on environmentally responsible chemical manufacturing has heightened interest in sustainable process design. Solvents contribute significantly to material consumption and waste generation in the chemical industry, making their selection a key factor in achieving sustainability. Green solvents provide a viable approach to reducing environmental impact while preserving process performance. This review critically analyzes the importance of green solvents in the design of sustainable chemical processes. Green solvents are solvents chosen or engineered to reduce environmental risks to promote health and safety impacts while preserving their effectiveness in chemical processes.

Unlike many traditional solvents that are volatile, toxic, or environmentally persistent, green solvents are characterized by lower toxicity, reduced vapor pressure, safer handling properties, and often renewable or biodegradable origins.

Scope of Green Solvents:

Green solvents represent a cornerstone of sustainable chemistry and environmentally responsible process engineering. Their scope extends beyond simple replacement of hazardous solvents; they reshape reaction design, separation strategies, safety protocols and lifecycle environmental performance. The concept originates from the principles of green chemistry, which prioritize minimizing toxicity, waste, energy consumption, and ecological harm. Traditional organic solvents contribute substantially to Volatile organic compound (VOC) emissions, Air and water pollution; Occupational health hazards Persistent environmental residues. They also aim to mitigate low toxicity, reduced volatility, biodegradability and lower environmental persistence. Thus, their scope includes reducing atmospheric emissions, minimizing hazardous waste and improving process safety.

Green solvents, while sometimes associated with higher initial costs, often provide significant financial benefits when evaluated over the entire process lifespan. Their lower volatility and improved recoverability can substantially decrease solvent losses, reducing the need for frequent replacement and lowering raw material expenses.

Taxonomy of Green Solvents:

Green solvents encompass diverse chemical systems with distinct physicochemical and sustainability characteristics. A taxonomy helps organize these systems based on origin, structure, and operational behavior. Green solvents encompass a wide variety of alternative liquid media developed to minimize the environmental, health and safety impacts associated with conventional volatile organic solvents. From a chemical perspective, water and aqueous systems represent the most fundamental category, valued for their non-toxicity, abundance, non-flammability and compatibility with biological and catalytic processes. Advances in aqueous reaction engineering, including micellar catalysis and biphasic systems, have expanded the applicability of water beyond traditionally soluble substrates. Another important class comprises supercritical fluids, particularly supercritical carbon dioxide ($scCO_2$), which exhibits tunable density, low viscosity and excellent mass transfer properties.

Additional categories include ionic liquids (ILs), deep eutectic solvents (DESs) and bio-based solvents. Ionic liquids, composed entirely of ions, are characterized by negligible vapor pressure, high thermal stability and highly customizable solvent properties, making them attractive for catalysis, electrochemistry and separations. However, concerns regarding toxicity, synthesis cost and recyclability necessitate careful lifecycle evaluation.

Table 1: Major Categories of Green Solvents

Category	Examples	Key Advantages	Limitations / Challenges	Typical Applications
Water	Water	Non-toxic, non-flammable, abundant, unique hydrophobic effects	Limited solubility for hydrophobic compounds, corrosion	Biocatalysis, aqueous-phase reactions
Bio-Based Solvents	Ethyl lactate, γ-valerolactone (GVL), 2-MeTHF	Renewable origin, biodegradable, reduced carbon footprint	Feedstock sustainability, purification energy	Organic synthesis, extraction
Supercritical Fluids	Supercritical CO_2	Tunable solvating power, residue-free removal, low toxicity	High-pressure equipment, energy for compression	Extraction, particle formation
Ionic Liquids (ILs)	Imidazolium-based ILs	Negligible vapor pressure, thermal stability, tunable properties	Cost, viscosity, incomplete toxicity data	Catalysis, separations
Deep Eutectic Solvents (DES)	Choline chloride–urea mixtures	Low cost, simple preparation, potential biodegradability	Limited industrial data, viscosity issues	Extraction, electrochemistry
Switchable Solvents	CO_2-responsive amines	Reversible polarity/phase change enabling easy separation	System complexity, scale-up challenges	Separation processes, CO_2 capture

Impact of Green solvetnts:

Green solvents play a crucial role in advancing sustainable process design because solvents frequently dominate both the mass balance and environmental footprint of chemical operations. In many industrial processes, solvents account for the largest fraction of material usage and waste generation. Selecting solvents with reduced toxicity, lower volatility and improved biodegradability directly decreases hazardous emissions, occupational risks and downstream treatment burdens. Consequently, solvent choice is no longer considered a secondary formulation decision but a central design parameter influencing overall sustainability metrics.

One of the most significant contributions of green solvents lies in their influence on reaction performance. Solvent properties such as polarity, hydrogen-bonding ability, dielectric constant and viscosity affect reaction kinetics, equilibrium and selectivity. Appropriately chosen green solvents can stabilize transition states, enhance reagent solubility and improve catalyst efficiency. These effects may lead to higher yields, fewer side products and reduced raw material consumption. Improved reaction efficiency inherently lowers waste generation and energy demand, reinforcing process sustainability.

Energy efficiency represents another critical dimension impacted by solvent selection. Conventional solvents often require energy-intensive separation techniques, particularly distillation. Green solvents with favorable thermo physical properties, such as optimal boiling points or phase-switching behavior, can reduce energy consumption during recovery and purification. Additionally, alternative separation strategies such as membrane filtration, liquid–liquid extraction, or supercritical fluid separation become viable when paired with suitable solvent systems. Lower separation energy directly translates into reduced greenhouse gas emissions and operational costs.

The adoption of green solvents also enhances process safety and regulatory compliance. Many traditional solvents pose risks related to flammability, explosiveness and chronic toxicity. Replacing such solvents with safer alternatives reduces fire hazards, solvent losses through evaporation and worker exposure. Improved safety profiles can simplify plant design by reducing the need for extensive containment, ventilation and explosion-proof infrastructure. Looking ahead, the synergy between computational modeling, machine learning, and green chemistry is expected to accelerate solvent innovation. Predictive tools can screen solvent candidates based on solvation behavior, toxicity indicators and process compatibility before experimental validation.

Industrial Applications of Green solvents:

Green solvents have gained substantial traction across multiple industrial sectors due to their ability to improve environmental performance, process safety and operational efficiency. In pharmaceutical manufacturing, greener alternatives such as bio-based ethers, alcohols, and water are increasingly replacing chlorinated and high-VOC solvents, resulting in reduced emissions and safer working conditions. In extraction industries, supercritical CO_2 is widely used for decaffeination, essential oil recovery and natural product purification because it eliminates toxic solvent residues and enables tunable selectivity. Catalytic processes benefit from ionic liquids and deep eutectic solvents, which facilitate catalyst immobilization, enhanced selectivity and solvent recyclability. processing, electrochemistry, and biomass valorization, where they contribute to reduced waste generation, improved material efficiency, and lower lifecycle.

Barriers and Practical Implications of Green Solvents:

The integration of green solvents into industrial chemical processes is often constrained by a combination of technical, economic and regulatory barriers. From a technical standpoint, alternative solvents may exhibit physicochemical properties that differ substantially from conventional systems, including higher viscosity, altered polarity or distinct phase behavior. Such variations can influence reaction kinetics, heat and mass transfer, catalyst performance and separation efficiency, thereby requiring re-optimization of operating conditions and, in some cases, redesign of process equipment. Scale-up presents an additional challenge, as solvent effects observed at laboratory scale do not always translate directly to large-scale reactors and separation units. Despite these barriers, the practical implications of adopting green solvents can be substantial. Successful implementation often leads to improved safety through reduced flammability and lower vapor emissions, along with decreased environmental liabilities associated with hazardous waste and solvent losses. Operational benefits may include enhanced reaction selectivity, improved catalyst recyclability, simplified waste handling, and compatibility with energy-efficient separation technologies.

Future Perspectives of Green Solvents:

The future evolution of green solvents is expected to be driven by advances in molecular design, digital technologies and sustainability-oriented process engineering. The integration of computational chemistry, thermodynamic modeling and machine learning is increasingly enabling predictive screening of solvent candidates based on solvation behavior, reaction compatibility, toxicity indicators and environmental impact. These data-driven methodologies significantly reduce experimental effort and accelerate the development of solvents optimized for both performance and safety.

Conclusion:

Green solvents have become a fundamental component in the advancement of sustainable chemical process design. Given that solvents frequently account for a large proportion of material usage, energy demand, and environmental emissions, their careful selection offers substantial opportunities to reduce the ecological footprint of chemical manufacturing. The adoption of safer, low-toxicity, and renewable solvent systems contributes not only to decreased hazardous waste and emissions but also to improved operational safety and regulatory compliance. Strengthened collaboration between chemists, chemical engineers and industry stakeholders will be essential to translating laboratory innovations into viable industrial solutions.

Acknowledgment

I would like to express my sincere gratitude to all those who contributed to the successful completion of this review on Green Solvents and Their Impact on Sustainable Chemical Process Design.

I am deeply thankful to my guide/supervisor for their continuous support, valuable guidance, and insightful suggestions throughout the preparation of this review. Their expertise and encouragement were instrumental in shaping this work.

Financial support and sponsorship
Nil.

Conflicts of interest
The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030118

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19466200

DOI Link:
https://doi.org/10.5281/zenodo.19466200

Volume: 3

Issue: 1(I)

Pp. 83-87

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 12 Jan. 2026

Revised: 22 Jan. 2026

Accepted: 04 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Reddy, D. S. (2026). Sustainable Waste Management in India: Strategies and Solutions. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 83–87. https://doi.org/10.5281/zenodo.19466200

Sustainable Waste Management in India: Strategies and Solutions

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Abstract

Effective waste management strategies are essential for sustainable urban development. Rapid urbanization and population growth have led to an increase in waste generation in developing countries like India. Waste management in urban areas poses a major challenge to administration departments of metropolitan cities and municipalities. This article explains the current challenges and explores various waste management strategies that can be implemented to address these challenges. Implementation of the strict policies for waste segregation at the source, the establishment of efficient recycling systems, and the implementation of public awareness campaigns to educate citizens about waste reduction practices may be the effective solutions to waste management. Application of smart technology in waste management, establishment of waste to energy plants and digital platforms for waste tracking, is examined. Encouragement of community involvement and public-private partnerships in enhancing waste management efficiency is discussed.

Keywords: *Sustainable urban development, waste management, public-private-local bodies collaboration.*

Introduction

India is a rapidly developing country with a population exceeding 1.4 billion. Swift urbanisation, which is driven by population explosion and unemployment lead to significant challenges to governments in providing basic amenities and waste management facilities. Approximately 62 million tons of solid waste is generated annually, with urban areas contributing about 70% of the total waste (Ministry of Housing and Urban Affairs, 2022), posing severe environmental and public health issues if not managed effectively. This article discusses sustainable waste management strategies in India, involving the integration of both community engagement and technological application as essential components for success. As per the World Bank's estimation, waste generation may increase from 2.01 billion tonnes in 2016 to 3.40 billion tonnes in 2050. Approximately 33% of this waste is mismanaged through dumping in open area or burning, subsequently causing soil & air pollution, and health hazards (World Bank, 2021).

The Waste Management Landscape in India

Current Challenges:

1. Waste Collection and Segregation: As per a report of the Central Pollution Control Board (CPCB, 2021), only about 60% of the waste generated is collected by the municipalities/ municipal corporations. Most of the collected waste is not segregated into biodegradable (wet waste) and non-biodegradable (dry waste) categories. At domestic level waste is mixed mostly consisting of disposable plastic and kitchen waste. Domestic waste particularly in urban slums and encroached areas, remains uncollected and dumped or burnt in the open areas.

2. Recycling Infrastructure: Waste recycling facilities in India are few compared to global standards. Most of the domestic organic wet waste can be recycled to generate compost fertilizer, biogas, or biomass energy etc. Disposable plastic waste can be recycled to generate tiles, bricks, and fuel etc. The lack of established recycling plants and infrastructure facilities impedes the efforts to divert waste from landfills (World Bank, 2021).

3. Public Awareness and Participation: There is a general lack of motivation among citizens/authorities/politicians regarding waste segregation, recycling, and the environmental hazards of improper waste disposal. There should be strict rules regarding waste segregation and disposal by municipal authorities, and penalties to be imposed on those who violate the rules. At the same time, these authorities should organize awareness programs on waste segregation into organic (wet), plastic, glass, and electronic waste. Municipal authorities should install sufficient waste bins or dumping facilities at domestic level and also at restaurants, markets etc. for the disposal of segregated waste. There are a lot of animal (cow/buffalo/ lamb/ chicken) leftovers from slaughterhouses and mutton/chicken shops, which are carelessly dumped openly at the outskirts, pose a hygienic threat after decomposing.

Municipal authorities should monitor these practices and make them responsible for whoever does not follow the proper waste disposal protocols and should impose penalties.

4. Policy and Regulatory Gaps: Though India has made various policies, such as the Solid Waste Management Rules (2016), but in practice its implementation is neglected, and many municipalities lack the capacity to implement these regulations effectively (Ministry of Environment, Forest and Climate Change, 2016).

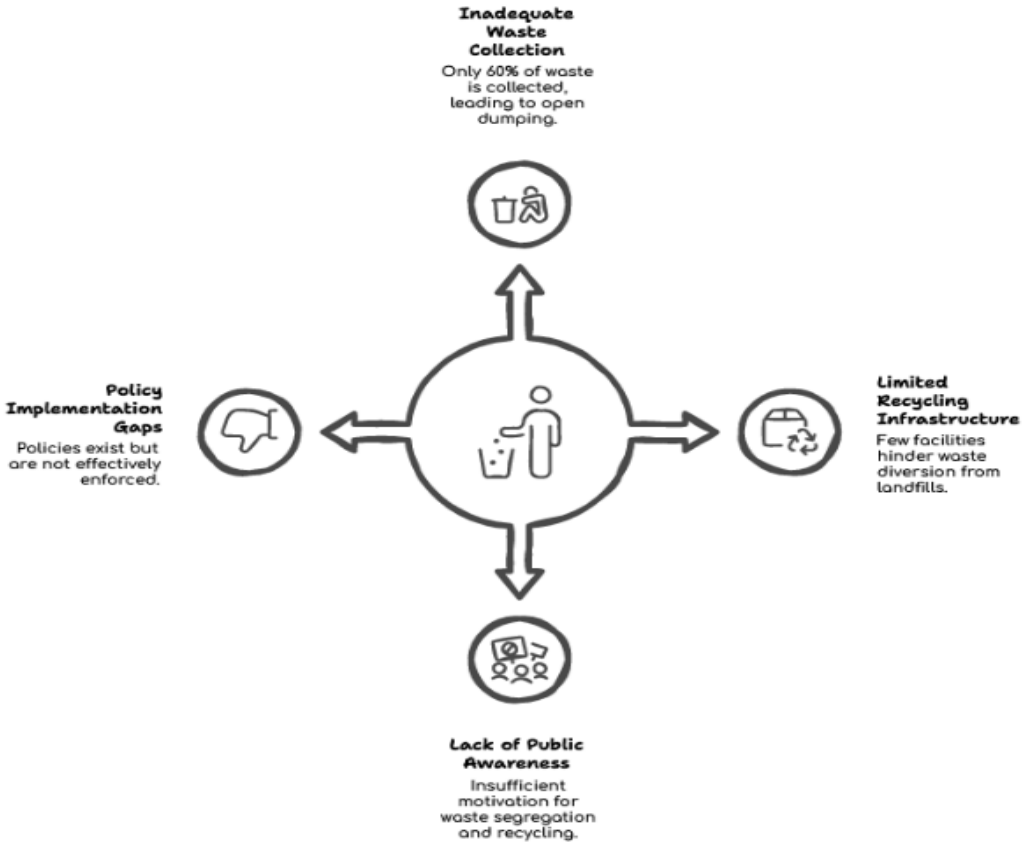


Figure: Waste management challenges in India

The Need for Sustainable Strategies and Solutions

To address the above challenges, the Indian government/state governments must adopt sustainable waste management policies by making use of technological advancements and community engagement. Sustainable waste management involves practices that minimize waste generation, promote reuse, recycling, and composting, and ensure safe disposal of residual waste at individual level. These policies are essential for protecting public health, conserving natural resources, and reducing environmental pollution.

1. **The Role of Community Engagement in Waste Management**

Community engagement is fundamental to the success of waste management initiatives. When communities are actively involved, they are more likely to adopt sustainable practices, leading to improved waste segregation, recycling, and overall waste reduction. Engaging communities fosters a sense of ownership and responsibility towards waste management, ultimately resulting in more effective and sustainable outcomes (Mansoor et al., 2019).

i. Awareness and Education Campaigns: Public awareness campaigns involving public and private volunteer organizations can educate individuals about the importance of waste segregation, recycling, and waste disposal. These campaigns may utilize various platforms, including social media, workshops, awareness weeks, and community meetings, similar to traffic awareness programs, to reach diverse individuals (Jain et al., 2020).

ii. Participatory Planning: Involving community members in the planning and decision-making policies related to waste management may generate more effective and specific solutions. Collaboration between local municipal authorities and resident communities by considering the needs and preferences of the community will be more effective (Bhatia et al., 2021).

iii. Incentive-based initiatives: Organising community-led initiatives, such as neighbourhood clean-up drives and waste segregation competitions, can motivate residents to take an active role in waste management. Felicitating the individuals with the highest participation with awards and proposing incentives and municipal tax waivers to residence communities can further enhance community participation (Kumar et al., 2022).

iv. Formation of Waste Management Committees: Establishing local waste management committees can empower resident communities/local bodies to take charge of waste management efforts. These committees can

bridge the gap between residents and local municipal authorities, ensuring that community concerns are addressed (Srinivasan et al., 2020).

2. **Case Studies of Successful Community Engagement**

Several cities have successfully implemented community engagement strategies in waste management:

i. Bangalore: The "Swachh Bangalore" initiative encouraged residents to segregate waste at the source and promoted composting of organic waste. The city saw significant improvements in waste segregation rates, with community participation playing a crucial role (Bangalore Solid Waste Management, 2020).

ii. Pune: Pune Municipal Corporation established waste management committees in various neighbourhoods, allowing residents to actively participate in waste management decisions. This approach resulted in increased awareness and improved waste segregation practices (Pune Municipal Corporation, 2021).

Technological Applications in Waste Management

1. The Role of Technology

Using technology is useful for enhancing the efficiency and effectiveness of waste management systems. Advanced technologies increase the efficiency rate of waste collection, improve recycling processes, and facilitate data-driven decision-making. The integration of technology in waste management can lead to reduced operational costs, increased recycling rates, and improved environmental outcomes (Sharma et al., 2021).

Key Technological Applications

i. Waste-to-Energy Technologies: Waste-to-energy (WtE) technologies convert biomass waste into usable energy, reducing the amount of waste sent to landfills. These technologies can help address the dual challenges of waste disposal and energy generation (Kumar et al., 2020).

ii. Digital Waste Tracking Systems: Implementing digital platforms like GPS-linked waste tracking can enhance accountability in waste management. These systems allow municipalities to track waste collection and monitor disposal processes, ensuring compliance with regulations (Gupta et al., 2021).

iii. Smart Bins and IoT Solutions: Smart waste bins equipped with sensors can monitor waste levels and manage collection routes, reducing operational costs and improving service efficiency. Automated waste collection vehicles, which have been used in western countries, effectively reduce contamination and infections to the municipal staff. The Internet of Things (IoT) facilitates both real-time data collection and projection & analysis of waste generation. Based on the analysis, the number of waste collection vehicles required, and waste recycling facilities needed may be estimated to make informed decisions (Rathore et al., 2022).

iv. Recycling Technologies: Advanced recycling technologies, such as automated waste segregation systems and chemical/organic-based recycling processes, can improve the efficiency of recycling operations. These technologies can help increase recycling rates and reduce contamination in recyclable materials (Sharma et al., 2020).

2. Case Studies of Technological Application

Several cities in India have successfully implemented technological applications in waste management:

i. Delhi: The Municipal Corporation of Delhi introduced smart waste bins that use sensors to monitor waste levels. This technology optimized waste collection routes, reducing operational costs and improving service delivery (Delhi Municipal Corporation, 2021).

ii.Ahmedabad: Ahmedabad municipal corporation implemented a waste biomass-to-energy plant that converts municipal solid waste biomass into electricity. This initiative has not only reduced the volume of waste sent to landfills but also provided a sustainable energy source for the city (Ahmedabad Municipal Corporation, 2020).

Integrating Community Engagement and Technological Applications

The Synergy Between Community and Technology

Integrating community engagement with technological application can lead to more effective waste management solutions. Advanced technology simplifies the tasks of resident communities and encourages them to participate actively in waste management efforts.

1. Strategies for Integration

i. Community Training Programs: Providing training programs that educate community members about new technologies can facilitate their effective use. This can include workshops on using digital waste tracking systems or operating smart bins (Nair et al., 2021).

ii. Feedback Mechanisms: Establishing feedback mechanisms that allow community members to report issues related to waste management can help municipalities identify areas for improvement. Technology can facilitate this process through mobile applications or online platforms (Verma et al., 2020).

iii. Collaborative Projects: Encouraging collaborative projects between communities and technology providers can lead to innovative waste management solutions (Desai et al., 2022).

iv. Public-Private Partnerships: Promoting public-private partnerships through Corporate Social Responsibility funds can facilitate the integration of community engagement and application of technology in waste management. These partnerships can leverage the strengths of both sectors to develop sustainable solutions (Kumar et al., 2021).

2. Case Studies of Successful Integration

i. Chennai: In Chennai, with the collaboration between local NGOs and technology firms, a mobile application was developed that allows residents to report waste management issues to the municipality. This initiative improved communication between local communities and municipal authorities, resulting in more efficient waste management (Chennai Municipal Corporation, 2021).

ii. Hyderabad: A public-private partnership pilot model that integrates community engagement with technological application was undertaken by Hyderabad Municipal Corporation. The partnership facilitated the introduction of smart waste bins and public awareness campaigns, leading to improved waste segregation and recycling rates (Hyderabad Municipal Corporation, 2020). In Malaysian township, KPHB the community association established sewage waste treatment plant and treated water is utilized to water the trees in the township.

Policy Framework for Sustainable Waste Management

Current Policies and Regulations

The Indian government made various policies and regulations aimed at improving waste management, including the Solid Waste Management Rules (2016) and the National Policy on Solid Waste Management (2000). However, enforcement and implementation remain ineffective.

Recommendations for Policy Improvement

1. **Strengthening Regulatory Authorities:** Policymakers should strengthen regulatory authorities for the effective enforcement and implementation of waste management regulations. This includes imposing penalties for non-compliance and providing incentives for municipalities and local communities that achieve waste management targets (Ministry of Environment, Forest and Climate Change, 2016).
2. **Promoting Decentralized Waste Management:** Encouraging decentralized waste management systems can empower communities to manage their waste more effectively. This approach can reduce the burden on centralized systems and promote local solutions (Srinivasan et al., 2020).
3. **Supporting Research and Development:** Investing in research and development for innovative waste management technologies supported by industry contributions can enhance the effectiveness of waste management systems. Funding for start-ups and research institutions can drive innovation in this sector (Nizami et al., 2020).
4. **Enhancing Capacity Building:** Training programs and workshops can equip stakeholders with the knowledge and skills needed to implement sustainable waste management practices (Bhatia et al., 2021).

Conclusion

Waste management is the responsibility of each individual. Sustainable waste management in India needs a collaborative approach that integrates community engagement and technological application. By encouraging communities to take an active role in waste management and to utilize technology to enhance efficiency, India can develop effective and sustainable waste management systems. Policymakers, municipal authorities, and local communities must collectively create an environment that encourages responsible waste management practices. Through these efforts, India can address its waste management challenges posed by rapid urbanisation and move towards a more sustainable future.

Acknowledgment

I would like to express my sincere gratitude to all those who contributed to the successful completion of this work on Sustainable Waste Management in India: Strategies and Solutions.

I am deeply thankful to my guide/supervisor for their continuous guidance, valuable suggestions, and constant encouragement throughout the course of this study. Their insights were instrumental in shaping this work.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| *Volume-3 Issue-1(I)* | *February-2026* | *ISSN: 3066-0637* | *Website:* https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030119

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19466681

DOI Link:
https://doi.org/10.5281/zenodo.19466681

Volume: 3

Issue: 1(I)

Pp. 88-91

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 12 Jan. 2026

Revised: 22 Jan. 2026

Accepted: 04 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Shekhar, V., Narsimha, D. B., Pingili, U., Kurapati, R., & Kommu, N. (2026). 1-Butyl-1-methylpyrrolidinium-1,2,4-triazolide ([BMP][Tz]): A Novel Ionic Liquid Solvent for Catalyst-Free N-tert-Boc Protection of Amines under Mild Conditions. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 88–91.
https://doi.org/10.5281/zenodo.19466681

1-Butyl-1-methylpyrrolidinium-1,2,4-triazolide ([BMP][Tz]): A Novel Ionic Liquid Solvent for Catalyst-Free N-tert-Boc Protection of Amines under Mild Conditions

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Abstract

We report the application of a newly synthesized ionic liquid, 1-butyl-1-methylpyrrolidin-1-ium 1H-1,2,4-triazol-1-ide [BMP][Tz], as a reaction medium for the solvent-assisted, N-tert-butoxycarbonylation of amines without a catalyst. A wide variety of structurally distinct amines, such as aryl, benzylic, secondary, and primary variations — reacted smoothly with Boc-anhydride (Boc2O) at ambient temperature to furnish the corresponding N-tert-butylcarbamates in yields ranging from high to excellent (95–98%). No additional catalyst or base was required. The ionic liquid [BMP][Tz] proved recyclable, retaining full catalytic activity across five consecutive reaction cycles.

Keywords: *[BMP][Tz]; ionic liquid; amine protection; N-Boc protection; Boc2O.*

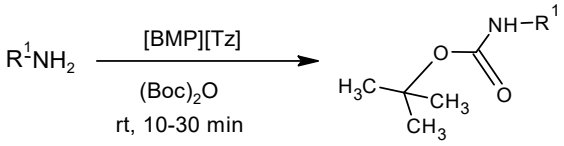
Introduction

The creation of ecologically friendly synthetic strategies has become a central objective of modern organic chemistry. Ionic liquids (ILs) are salts that dissolve at temperatures lower than 100°C. They have attracted considerable attention as sustainable alternatives to traditional organic volatile solvents[1]. Their distinctive attributes, such as a wide range of liquid temperatures, non-flammability, and minimal vapor pressure, and inherent chemical stability, make them particularly attractive for green chemistry applications[2]. A further advantage is their tunability: the physicochemical properties of an IL may be adjusted by means of the systematic change of. Choosing the proper cation anion pairs, which qualify them the name of designer. A subdivision, task-specific ionic liquids (TSILs), has been designed in such a way as to fulfil meaning either catalytic or reactive functions in a single medium[3]. In theory diverse range of potential ionic liquids has more than 10^{18} combinations, a few hundred. are already available in the market[4]

Several synthetic routes to novel ILs via straightforward acid–base neutralisation have been described in the literature. Notable examples include the preparation of Brønsted acid-base ILs from bis (trifluoro methane sulfonyl) amide and imidazole[5,6], a family of guanidinium-based ILs obtained by neutralising 1,1,3,3-tetramethylguanidine with various protic acids[5], and chiral ILs derived from quaternary ammonium hydroxides paired with carboxylic acids[7]. Despite these advances, the preparation of chiral ILs from inexpensive, readily available precursors remains underexplored.

Among the many functional groups encountered in target-directed synthesis, the *tert*-butyloxycarbonyl (Boc) group occupies a pivotal role as a protecting group for amines[8]. Boc-carbamates display excellent stability under basic and nucleophilic conditions yet are cleanly and selectively cleaved to regenerate in somewhat acidic environments the free amine. When triethylamine is present as a base, conventional Boc-protection relies on an amine's interaction with di-tert-butyl dicarbonate (Boc_2O) using anhydrous dichloromethane as solvent[9–15]. Variants employing 4-(dimethylamino) pyridine (DMAP) as acylation catalyst[16], Boc-imidazole as a transfer reagent[17], or *tert*-butoxycarbonyl-1,2-dihydroisoquinoline[18] have also been described. Despite the availability of diverse base-mediated and Lewis acid-catalysed protocols, this work has been accomplished using an ionic liquid as the reaction media in a catalyst-free manner. In the course of our ongoing programme on IL-mediated organic transformations, we prepared the novel pyrrolidinium-based ionic liquid 1-butyl-1-methyl pyrrolidinium-1,2,4-tri azolide([BMP][Tz]). Herein, we describe the utility of [BMP][Tz] as a productive, reusable reaction media for the smooth and catalyst-free *N-tert*-butoxycarbonylation shows a panel of amines with a variety of structures at ambient temperature.

Results and Discussion

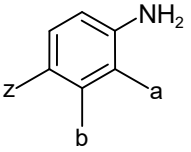
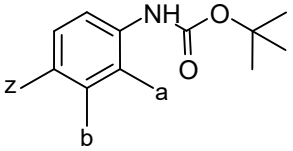
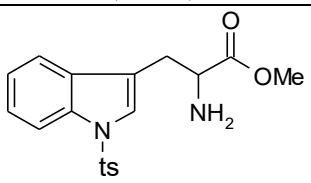
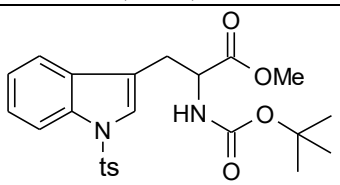
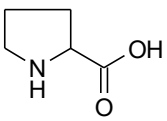
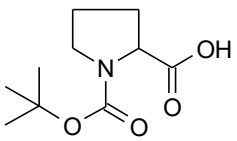


Scheme 1

Initial optimisation studies established that [BMP][Tz] serves as an effective reaction medium for Boc-protection without the need for any added catalyst or base (Scheme 1). The reaction proceeds under operationally simple conditions: no inert atmosphere or anhydrous precautions are required, and no detectable by-products are formed. As a benchmark experiment, Boc_2O (1.2 mmol) was used to treat aniline (1 mmol) in [BMP][Tz] at 25 °C. The corresponding *N*-phenyl carbamate was separated with a result of yield 98% within 10 min (entry 1 in table 1), demonstrating the high reactivity of the system. This outcome emboldened the extent of the response was analyzed throughout an electronically and sterically diverse collection of aryl amines, benzylic amines, primary amines, secondary amines, and (Table 1)

All substrates were cleanly and readily converted to the desired as summarised in Table 1. The yield of the N-Boc products is 95-98 percent isolated. There are electron-withdrawing substituents. The reaction times were short and the aryl methoxy carbonyl) on the ring was well tolerated. Secondary and benzylic amines also were accommodated. efficiently. These results prove that [BMP][Tz] offers very favourable results. Micro environment of the reaction, by postulating to stabilize the transition state presumably. ion and hydrogen-bond with the carbonyls. The ionic liquid was recovered by isolation, by aqueous workup and ethyl acetate extraction. the water phase and recycled without significant efficiency decreases in five consecutive cycles, emphasizing the recyclability of the medium in reality.

Table 1. Scope of *N-tert*-butoxycarbonylation of amines in [BMP][Tz].[a]

Entry	Substrate	Product	Time(min)	Yield (%)
				
A	a = H, b = H, z = H	a= H, b = H, z = H	12	98
B	a = H, b = NO_2, z = H	a = H, b= NO_2, z = H	16	96
C	a = H, b = H, z = NO_2	a = H, b = H, z = NO_2	12	98
D	a = H, b = H, z = OH	a = H, b = H, z = OH	14	96
E	a = H, b= H, z = OAc	a = H, b= H, z = OAc	20	97
F	a = CH_3, b = H, z = H	a= CH_3, b = H, z = H	25	95
G	a = H, b = H, z = F	a = H, b = H, z = F	25	95
H	a= COOMe, b = H, z = H	x = COOMe, b= H, z = H	8	97
I			15	96
J			15	95

All the reactions were done at room temperature using Boc_2O (1.2 mmol) per mmol amine in BMP] [Tz] (1 mL). Yields are detached products that are defined by ^1H NMR and EIMS.

Conclusion

Using, a mild, catalyst-free procedure to the N-Boc protection of amines is developed. the benign and recyclable reaction medium ionic liquid [BMP][Tz] at room temperature, does not require a base or catalyst, and can tolerate a wide variety of amine. Substrates, and provided N-tert-butylcarbamates in high yields and short reaction times. The process of being able to recover the ionic liquid and be able to reuse it several times with no degradation. This methodology is a useful supplement to already available Boc-protection, especially by the aspect of green and sustainable synthesis.

Experimental

Every reagent and solvent employed was analytically pure and didn't require any additional purification, unless otherwise noted. TLC was used to monitor the reactions that were evident under a UV lamp. ^{1}H NMR spectra in $CDCl_3$ were recorded using 300 MHz spectrometer; ^{1}H NMR vallues (δ) are given in ppm. in relation to TMS. Mass spectra was acquired by (EIMS) on an Elegant LC-1100 series instrument.

2. Synthesis of N-tert-Butylcarbamates: General Procedure

In an open glass vial, Boc_2O [1.2 mmol] and the amine substrate [1.0 mmol] were dissolved in [BMP][Tz][1.0 mL]. At 25°C, or room temperature, the mixture was magnetically agitated until TLC appeared that all of the initial supplies had been utilized. (see Table 1 for reaction timings). After adding 5 mL of distilled water, the product was taken out utilizing 3 × 20 mL ethyl acetate. Mixture of organic extracts was dried over the anhydrous Na_2SO_4 after being cleaned with saturated aqueous NaCl (brine, 20 mL).Four. Pure N-tert-butylcarbamate was obtained by employing column chromatography to purify the crude product after solvent removal at low pressure. The remaining aqueous phase was concentrated to recover [BMP][Tz] under lower pressure, which was dried at 60 °C under vacuum and reused directly in subsequent runs. For at least five consecutive cycles, the ionic liquid maintained full activity.

3. Spectral Data:

Product A: White solid; MS- m/z 194 [M]$^+$. ^{1}H NMR): δ 7.35 (4H, m), 7.05 (1H, J = 7.1 Hz, t), 6.35 (1H, br s, NH), 1.52 (9H, s). mp 134°C.

Product B: White solid; MS- m/z 238 [M]$^+$. ^{1}H NMR: δ 8.65 (1H, m), 7.81–7.96 (2H, m), 7.6(1H, J = 7.1 Hz, t), 1.5 (9H, s), mp 93.5°C.

Product C: White solid; MS- m/z 238 [M]$^+$. ^{1}H NMR: δ 8.2 (2H, J = 6.6 Hz,d), 7.6 (2H, J = 6.6 Hz, d), 1.52 (9H, s). mp 112.5°C.

Product D: White solid; MS- m/z 209 [M]$^+$. ^{1}H NMR: δ 7.10 (2H, J = 7.2 Hz, d), 6.72 (2H, J = 7.2 Hz, d), 6.26 (1H, br s, NH), 4.77 (1H, br s, OH), 1.52 (9H, s,). mp 142°C

Product E: White solid; MS- m/z 251 [M]$^+$. ^{1}H NMR: δ 7.65 (2H, J = 7.2 Hz, d), 7.05 (2H, J = 7.2 Hz, d), 5.92 (1H, br s, NH), 2.12 (3H, s), 1.52 (9H, s); mp 111°C

Product F: White solid; MS- m/z 207. ^{1}H NMR: δ 7.81 (1H, d), 7.26-7.02 (2H, m), 6.91 (m, 1H), 6.21 (1H, br s, NH), 2.26 (3H, s), 1.52 (9H, s). mp 82.6°C

Product G: White solid; ^{1}H NMR: δ 7.41 (2H, m), 7.12 (2H, m), 5.61 (1H, br s, , NH), 1.52 (9H, s). mp 125.5°C

Product H: White solid; MS- m/z 251 [M]$^+$. ^{1}H NMR: δ 8.22 (1H, m), 8.13 (m, 1H), 7.60 (1H, m,), 6.92 (1H, m), 5.11 (1H, br s, NH), 1.52 (9H, s). mp 111.5°C.

Product I: White solid; MS- m/z 472 [M]$^+$. ^{1}H NMR: δ 8.31 (1H, m), 8.05 (1H, m), 7.82 (m, 1H), 7.72 (m, 2H), 7.35 (1H, s), 7.31 (m, 1H), 7.11 (2H, m), 4.51 (1H, br s, NH), 4.41 (1H,m), 3.68 (3H, s), 3.33–3.51 (2H, m), 1.44 (9H, s). mp 54.5°C.

Product J: White solid; MS- m/z 215 [M]$^+$. ^{1}H NMR: δ 9.05 (1H, br s, NH), 4.41 (m, 1H), 3.41 (2H, m), 2.12 (m, 4H), 1.41 (9H, s). mp 123.5°C.

Acknowledgements

The authors highly appreciate the Government Degree College, Hayathnagar, and the. Analytical and access to analytical is available in Indian Institute of Chemical Technology, Hyderabad.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030120

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19466782

DOI Link:
https://doi.org/10.5281/zenodo.19466782

Volume: 3

Issue: 1(I)

Pp. 92-94

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 12 Jan. 2026

Revised: 22 Jan. 2026

Accepted: 04 Feb. 2026

Published: 28 Feb 2026

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How to cite this article:
Sudha, Y. C. (2026). Narrative Alchemy: Transmuting Text through Chemical Lenses. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 92–94.
https://doi.org/10.5281/zenodo.19466782

Narrative Alchemy: Transmuting Text through Chemical Lenses

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Abstract

This paper proposes an interdisciplinary interpretive framework titled 'Narrative Alchemy,' which examines literary texts through conceptual parallels drawn from chemistry and environmental sciences. While literature and chemistry are often treated as separate intellectual territories, both disciplines are deeply concerned with transformation, interaction, and systemic balance. By employing chemical principles such as reaction, catalysis, synthesis, entropy, and equilibrium, this study develops a model of chemical hermeneutics that reimagines narrative as a dynamic system. The paper aligns this framework with environmental thought by treating texts as ecosystems where characters, ideas, and contexts interact within structured yet evolving networks. Such an approach foregrounds process rather than static meaning and highlights how narrative change resembles material transformation in natural systems. The interdisciplinary method demonstrates relevance to environmental humanities and sustainability studies by showing how literary analysis can adopt scientific metaphors responsibly and productively.

Keywords: *Narrative Alchemy; Chemical Hermeneutics; Environmental Humanities; Entropy; Equilibrium; Interdisciplinary Studies*

Introduction

Interdisciplinary scholarship increasingly demonstrates that meaningful insight emerges at the intersections of disciplines. Chemistry studies matter and its transformations, while literature explores human experience through symbolic representation. Despite methodological differences, both domains share a commitment to understanding change. Storytelling converts lived experience into structured meaning, much as chemical reactions convert substances into new compounds. This paper argues that chemical principles offer structurally illuminating models for interpreting narrative systems. By conceptualizing text as a dynamic environment, we uncover parallels between ecological balance and literary structure. Interdisciplinary scholarship increasingly demonstrates that meaningful insight emerges at the intersections of disciplines. Chemistry studies matter and its transformations, while literature explores human experience through symbolic representation. Despite methodological differences, both domains share a commitment to understanding change. Storytelling converts lived experience into structured meaning, much as chemical reactions convert substances into new compounds. This paper argues that chemical principles offer structurally illuminating models for interpreting narrative systems. By conceptualizing text as a dynamic environment, we uncover parallels between ecological balance and literary structure. Interdisciplinary scholarship increasingly demonstrates that meaningful insight emerges at the intersections of disciplines. Chemistry studies matter and its transformations, while literature explores human experience through symbolic representation. Despite methodological differences, both domains share a commitment to understanding change. Storytelling converts lived experience into structured meaning, much as chemical reactions convert substances into new compounds. This paper argues that chemical principles offer structurally illuminating models for interpreting narrative systems. By conceptualizing text as a dynamic environment, we uncover parallels between ecological balance and literary structure.

Conceptual Foundations of Chemical Hermeneutics

Hermeneutics refers to the theory of interpretation. Chemical hermeneutics extends this concept by understanding texts as systems of interaction. In chemistry, reactions depend upon concentration, temperature, pressure, and catalysts. Similarly, narrative meaning depends upon historical context, cultural forces, genre conventions, and reader participation. Meaning is emergent rather than fixed. It arises from relationships among narrative elements, not from isolated components. This systemic perspective aligns closely with environmental sciences, where ecosystems function through interdependent relationships. Hermeneutics refers to the theory of interpretation. Chemical hermeneutics extends this concept by understanding texts as systems of interaction.

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Reaction and Narrative Conflict

Chemical reactions require activation energy. In narrative, conflict serves this catalytic role. Without tension, the story remains static. The introduction of opposing forces destabilizes equilibrium and initiates transformation. Characters function as reactive agents whose interactions produce new narrative configurations. Like exothermic reactions, dramatic confrontations release emotional intensity, reshaping the textual environment. Chemical reactions require activation energy. In narrative, conflict serves this catalytic role. Without tension, the story remains static. The introduction of opposing forces destabilizes equilibrium and initiates transformation. Characters function as reactive agents whose interactions produce new narrative configurations. Like exothermic reactions, dramatic confrontations release emotional intensity, reshaping the textual environment. Chemical reactions require activation energy. In narrative, conflict serves this catalytic role. Without tension, the story remains static. The introduction of opposing forces destabilizes equilibrium and initiates transformation. Characters function as reactive agents whose interactions produce new narrative configurations. Like exothermic reactions, dramatic confrontations release emotional intensity, reshaping the textual environment.

Catalysis and Narrative Acceleration

A catalyst accelerates reaction without being consumed. In storytelling, minor characters or pivotal events often perform catalytic functions. A single encounter may transform a protagonist's trajectory without altering the catalyst itself. This principle mirrors ecological phenomena where minor disturbances trigger large systemic changes. Understanding catalysis clarifies structural economy within narrative design. A catalyst accelerates reaction without being consumed. In storytelling, minor characters or pivotal events often perform catalytic functions. A single encounter may transform a protagonist's trajectory without altering the catalyst itself. This principle mirrors ecological phenomena where minor disturbances trigger large systemic changes. Understanding catalysis clarifies structural economy within narrative design. A catalyst accelerates reaction without being consumed. In storytelling, minor characters or pivotal events often perform catalytic functions. A single encounter may transform a protagonist's trajectory without altering the catalyst itself. This principle mirrors ecological phenomena where minor disturbances trigger large systemic changes. Understanding catalysis clarifies structural economy within narrative design.

Entropy, Disorder, and Environmental Instability

Entropy refers to the tendency toward disorder within closed systems. Narratives frequently depict fragmentation, decay, or moral collapse—forms of textual entropy. Yet storytelling simultaneously resists disorder by imposing structure and coherence. This tension between chaos and order parallels environmental systems struggling between degradation and resilience. Viewing narrative through thermodynamic analogy highlights instability as a generative force. Entropy refers to the tendency toward disorder within closed systems. Narratives frequently depict fragmentation, decay, or moral collapse—forms of textual entropy. Yet storytelling simultaneously resists disorder by imposing structure and coherence. This tension between chaos and order parallels environmental systems struggling between degradation and resilience. Viewing narrative through thermodynamic analogy highlights instability as a generative force. Entropy refers to the tendency toward disorder within closed systems. Narratives frequently depict fragmentation, decay, or moral collapse—forms of textual entropy. Yet storytelling simultaneously resists disorder by imposing structure and coherence. This tension between chaos and order parallels environmental systems struggling between degradation and resilience. Viewing narrative through thermodynamic analogy highlights instability as a generative force.

Equilibrium and Narrative Resolution

Chemical equilibrium represents dynamic balance rather than static rest. Reactions continue in opposing directions at equal rates. Similarly, narrative resolution often suggests provisional balance rather than permanent harmony. Underlying tensions may persist even after apparent closure. This interpretation reframes endings as stabilized transformations within evolving systems. Chemical equilibrium represents dynamic balance rather than static rest. Reactions continue in opposing directions at equal rates. Similarly, narrative resolution often suggests provisional balance rather than permanent harmony. Underlying tensions may persist even after apparent closure. This interpretation reframes endings as stabilized transformations within evolving systems. Chemical equilibrium represents dynamic balance rather than static rest. Reactions continue in opposing directions at equal rates. Similarly, narrative resolution often suggests provisional balance rather than permanent harmony. Underlying tensions may persist even after apparent closure. This interpretation reframes endings as stabilized transformations within evolving systems.

Synthesis and Intertextual Ecology

Synthesis combines elements into more complex compounds. Literary texts similarly synthesize myths, genres, and cultural memories. Intertextuality operates as a form of cultural chemistry, generating layered meaning. In eco-literature, natural imagery and scientific vocabulary blend with ethical reflection, forming interdisciplinary compounds of knowledge. Synthesis combines elements into more complex compounds. Literary texts similarly synthesize myths, genres, and cultural memories. Intertextuality operates as a form of cultural chemistry, generating layered meaning. In eco-literature, natural imagery and scientific vocabulary blend with ethical reflection, forming interdisciplinary compounds of knowledge. Synthesis combines elements into more complex compounds. Literary texts similarly synthesize myths, genres, and cultural memories. Intertextuality operates as a form of cultural chemistry, generating layered meaning. In eco-literature, natural imagery and scientific vocabulary blend with ethical reflection, forming interdisciplinary compounds of knowledge.

Environmental Humanities and Narrative Systems

The environmental humanities emphasize interconnectedness between human culture and natural systems. By treating narrative as ecosystem, we highlight interdependence among characters, themes, and settings. Each narrative element contributes to systemic balance. This ecological model encourages sustainable thinking and systemic awareness. The environmental humanities emphasize interconnectedness between human culture and natural systems. By treating narrative as ecosystem, we highlight interdependence among characters, themes, and settings. Each narrative element contributes to systemic balance. This ecological model encourages sustainable thinking and systemic awareness. The environmental humanities emphasize interconnectedness between human culture and natural systems. By treating narrative as ecosystem, we highlight interdependence among characters, themes, and settings. Each narrative element contributes to systemic balance. This ecological model encourages sustainable thinking and systemic awareness.

Methodological Implications

Applying chemical lenses to literature fosters collaborative research between scientists and humanists. It demonstrates how metaphor can function as analytical bridge without oversimplification. The model encourages cross-disciplinary pedagogy and sustainability-focused scholarship. Applying chemical lenses to literature fosters collaborative research between scientists and humanists. It demonstrates how metaphor can function as analytical bridge without oversimplification. The model encourages cross-disciplinary pedagogy and sustainability-focused scholarship. Applying chemical lenses to literature fosters collaborative research between scientists and humanists. It demonstrates how metaphor can function as analytical bridge without oversimplification. The model encourages cross-disciplinary pedagogy and sustainability-focused scholarship.

Conclusion

Narrative alchemy conceptualizes storytelling as transformative chemistry operating within environmental systems of meaning. Through reaction, catalysis, entropy, equilibrium, and synthesis, texts evolve as dynamic structures. This interdisciplinary framework aligns with environmental and earth studies by emphasizing systemic interdependence and balance. Transmuting text through chemical lenses ultimately reveals shared processes of transformation in both matter and meaning. Narrative alchemy conceptualizes storytelling as transformative chemistry operating within environmental systems of meaning. Through reaction, catalysis, entropy, equilibrium, and synthesis, texts evolve as dynamic structures. This interdisciplinary framework aligns with environmental and earth studies by emphasizing systemic interdependence and balance. Transmuting text through chemical lenses ultimately reveals shared processes of transformation in both matter and meaning. Narrative alchemy conceptualizes storytelling as transformative chemistry operating within environmental systems of meaning. Through reaction, catalysis, entropy, equilibrium, and synthesis, texts evolve as dynamic structures. This interdisciplinary framework aligns with environmental and earth studies by emphasizing systemic interdependence and balance. Transmuting text through chemical lenses ultimately reveals shared processes of transformation in both matter and meaning.

Acknowledgment

I would like to express my sincere gratitude to all those who contributed to the successful completion of this work on Narrative Alchemy: Transmuting Text through Chemical Lenses.

I am deeply thankful to my guide/supervisor for their continuous encouragement, thoughtful guidance, and insightful perspectives that helped shape this interdisciplinary study. Their support was invaluable in bridging the domains of literature and chemistry.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| *Volume-3 Issue-1(I)* | *February-2026* | *ISSN: 3066-0637* | *Website:* https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030121

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

Creative Commons (CC BY-NC-SA 4.0)

DOI: 10.5281/zenodo.19466996

DOI Link: https://doi.org/10.5281/zenodo.19466996

Volume: 3

Issue: 1(I)

Pp. 95-102

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 14 Jan. 2026

Revised: 24 Jan. 2026

Accepted: 06 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Salwadi, Y., Venkatesham, K., Burri, V., Matkala, B., Boggala, S., & Aytam, H. P. (2026). Role of Si/Al ratio in the Valorization of Glycerol to a Fuel Additive, Solketal over HZSM-5 Catalysts. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 95–102. https://doi.org/10.5281/zenodo.19466996

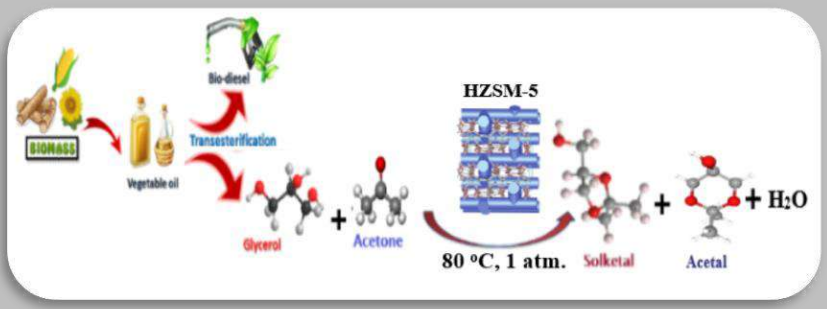
Role of Si/Al ratio in the Valorization of Glycerol to a Fuel Additive, Solketal over HZSM-5 Catalysts

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Abstract

Valorization of glycerol, a by-product of bio-diesel production is an inevitable process for its economic viability. The study on various zeolites showed HZSM-5 to be an effective and stable catalyst in the conversion of glycerol to solketal which motivated the present study in order to understand the role of Si/Al ratio on its catalytic activity. HZSM-5 catalysts with Si/Al ratios of 12:1, 30:1, 80:1 and 150:1 that have been modified to acidic form from ammonical form. All these catalysts were characterized by BET-SA, XRD, SEM-EDAX, FT-IR, Raman, XPS, TPD of NH_3 and Py adsorbed IR studies. The catalytic activity towards selective acetalization of glycerol to solketal was evaluated by varying the parameters viz., temperature, mole ratio of glycerol:acetone, catalyst amount and time on stream in order to understand the significance of Si/Al ratio of HZSM-5 catalysts. The optimized conditions of reaction parameters indicated a 100 mg catalyst, mole ratio of glycerol:acetone = 1:10, at 80 °C, ambient pressure and the lowest ratio of Si/Al = 12:1 of HZSM-5 to show higher activity (~ 14.5 mmol $h^{-1}g_{cat}^{-1}$) over its counterparts attributed to higher acidity as indicated from TPD of NH_3 and Ex-situ py-IR studies.

Keywords: *Glycerol, Solketal, Acetalization, Acidity, HZSM-5, Si/Al ratio*



Scheme: Glycerol valorization to solketal over HZSM-5 (12:1) catalyst

Introduction

Glycerol is a by-product generated in 10% of every batch of bio-diesel production in the industry [1]. Bio-diesel is gaining immense importance owing to its generation from renewable biomass resources since the fuels used till date extensively are from non- renewable resources that are expected to be extinct in near future [2]. And also, these fuels are highly polluting due to their greater carbon footprint. These fuels or petroleum-based feed stocks are a source of many bulk and fine chemicals in general and hence alternative renewable resources are at high demand in this regard as well [3]. Glycerol is also non-toxic, bio-compatible, cheaper and available in plenty that can be used a chemical feedstock [4]. Valorization of glycerol to solketal, a useful fuel additive, not only makes the bio-diesel production economical but also provides valuable chemicals syntheses via renewable biomass resources. Glycerol acetalization is an acid catalyzed reaction [5-10] and hence simple acidic zeolites studied with higher acidic sites showed effective transformation to solketal [11, 12]. Hence, HZSM-5 zeolites with variable Si/Al ratios were studied to understand the influence of Si/Al ratio that contributes to the enhancement in the acidity of the catalyst which in turn raised the solketal yields at mild reaction conditions. The results of these studies are presented in this chapter.

Experimental Methods

Chemicals Used: The reactants, glycerol and acetone were of Sigma Aldrich and Spectrochem make of AR grade respectively which were used as such in the reaction with no further treatment.

Preparation of Catalysts: Commercial ammonical form of ZSM-5 zeolites with variable Si/Al ratios of 12, 30, 80 and 150 were purchased from Alfa Aesar. These ammonical zeolites were calcined at 500 °C for 5 h to obtain their respective acidic zeolites.

Characterization Techniques: Powder X-ray diffraction (XRD) analysis was carried out on a Rigaku Miniplex X-ray diffractometer with Cu K_α (1.5406 Å) radiation source operated at 40kV and 15mA. N_2 adsorption, at -196 °C was measured over Micromeritic ASAP 2010 surface area analyzer and Scanning Electron Microscopy (FE-SEM) with Energy Dispersive X-ray (EDX) analyzer for elemental distribution was used to study the surface morphology of the catalysts. Thermo Nicolet iS50 with inbuilt ATR is used in recording FT-IR spectra of catalysts in the range of 400-4000 cm^{-1}. Raman Spectra were obtained using a 633 nm line from a He–Ne laser using HORIBA JOBIN YVON HR800, Japan instrument. Acidity measurements of catalysts were carried out by NH_3-TPD on an Auto Chem 2910 (Micromeritics). A KRATOS-AXIS 165 instrument with Mg K_α radiation source was used for XPS analysis of samples.

Activity evaluation of catalysts: Acetalization of glycerol to solketal was conducted in a batch type glass reactor closed with a septum placed over a magnetic stirrer under variable reaction conditions of temperature, catalyst amount and mole ratios of reactants in the reactor. At regular intervals of time the reaction mixture was collected and analysed by a GC (Agilent 1020A) equipped with a FID. The products were confirmed by GC-MS. The reaction mixture was centrifuged to separate the catalyst, washed with deionized water and dried in oven at 100 °C overnight in order to test the reusability of the catalysts. The conversion of glycerol (X) and selectivity to solketal (S) were obtained using the following equations: Conversion of Glycerol (X_{Gly}%): $\%X_{Gly} = \frac{C_{Gly_o} - C_{Gly}}{C_{Gly_o}} \times 100$

where C_{Gly_o} is the molar concentration (mol/L) of glycerol before the reaction and C_{Gly} is the molar concentration (mol/L) of glycerol after the reaction; Selectivity to Solketal (S_{Skt}%): $\%S_{Skt} = \frac{C_{Skt}}{C_{Gly_o} - C_{Gly}}$

where C_{Skt} is the molar concentration (mol/L) of solketal after the reaction.

Results and Discussion

XRD Results: X-ray diffractograms of HZSM5 catalysts with variable Si/Al ratios recorded are presented in figure 4.1. Characteristic diffraction peaks of MFI structure of these catalysts could be noticed from 2θ = 8.0°, 9.0°, 14.8°, 22.9°, 24.0° and 29.8° corresponding to (101), (200), (301), (501), (303) and (503) planes respectively [13]. The diffractograms clearly indicate the microcrystalline structure of ZSM5. The crystallite size as calculated using Scherrer equation indicate lower size with lower Al content/higher silica content though the specific surface area also lowered in the same order as presented in table 1. The peaks of HZSM-5 sample with higher Si/Al ratio of 150:1 showed slight broadening as compared to the rest of the samples probably due to increased Si content. ZSM-5 zeolite structure has bimodal pores with large no. of micropores (0.51-0.56 nm) and small no. of mesopores (about 3 nm) [14].

Table-1: Physico-chemical characteristics of HZSM-5 catalysts

HZSM-5 with Si/Al ratio	BET-SA (m^2g^{-1})		Crystallite size, nm (from XRD) in H-form
	NH_4-Form	H-Form	
12:1	400	370	35.5
30:1	384	360	23.1
80:1	362	354	22.0
150:1	355	342	19.5

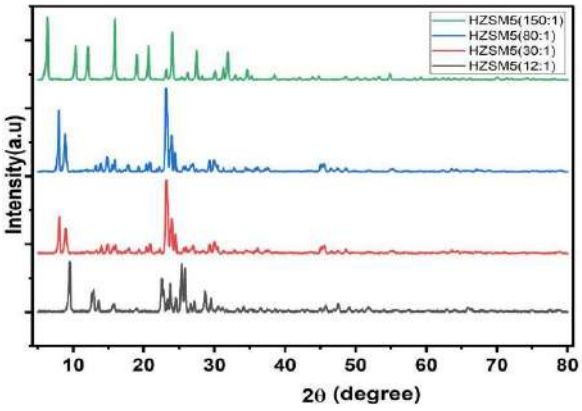
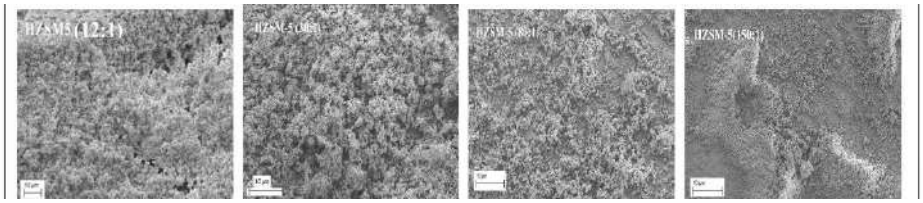


Figure 1: XRD patterns of HZSM-5 catalysts with varying Si/Al ratios

N_2 Adsorption studies: The specific surface areas of the HZSM-5 samples were measured by BET method, N_2 adsorption isotherms recorded (not shown here) for these catalysts with variable Si/Al ratios showed lowering of the surface area with the increase in the ratio as presented in table 1.



SEM-EDX results: The SEM images of the HZSM-5 catalysts with variable Si/Al ratios along with their elemental compositions obtained from EDX spectra are presented in the figure 4.2. The zeolite catalysts displayed a spherical morphology with well distributed particles and similar surface appearance. The particles seem to get agglomerated with the reduction in Si/Al ratio from 150:1 to 12:1. The particle size reduced with decrease in Al content. This correlates well with the decrease in crystallite size observed with increase in Si/Al ratio from XRD data as given in table 1. The elemental composition data also correlates well with the Si/Al ratio as evidenced from the decrease in Al composition from the catalysts with 12:1 to 150:1.

(A) HZSM-5 (12:1)			(B) HZSM-5 (30:1)			(C) HZSM-5 (80:1)			(D) HZSM-5 (150:1)		
Element	**Wt.**	**At.**	**Element**	**Wt.**	**At.**	**Element**	**Wt.**	**At.**	**Element**	**Wt.**	**At.**
	%	**%**		**%**	**%**		**%**	**%**		**%**	**%**
O K	57.5	70.2	O K	58.2	70.9	O K	53.3	66.3	O K	49.8	61.2
Si K	36.0	25.0	Si K	40.3	28.0	Si K	45.6	32.8	Si K	49.8	38.6
Al K	6.6	4.8	Al K	1.5	1.1	Al K	1.1	0.9	Al K	0.4	0.2
Total	**100**		**Total**	**100**		**Total**	**100**		**Total**	**100**	

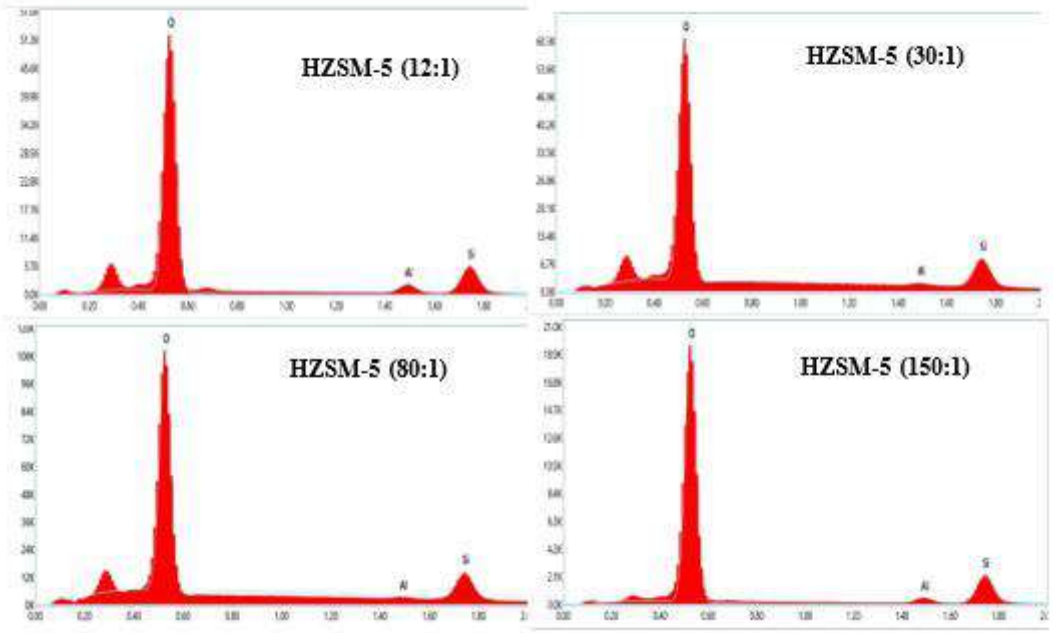


Figure 2: SEM-EDX of HZSM-5 catalysts with differet Si/Al ratios

FT-IR and Raman spectral results: The IR spectrum of MFI zeolite framework of ZSM-5 is expected to result in 323 active fundamental IR modes and 432 fundamental modes of Raman associated to the unit cell of large dimension comprising of 288 atoms among which are 96 Si or Al tetrahedral atoms (T) and 182 oxygen atoms. But most of the vibrational modes are superimposed owing to similar atomic positions, bond lengths and angles [15]. A very strong T–O–T asymmetric stretching vibrational mode centered at 1102 cm^{-1} along with a shoulder seen from fig. 3 at 1221 cm^{-1} while its symmetric stretching band at 796 cm^{-1} was found to be weaker. The deformation modes of T–O–T viz., a weak in-plane bending and a strong out of plane rocking mode of vibration at 454 cm^{-1} are also seen in the IR spectra of HZSM 5 zeolites that are typical of the MFI structure [16, 17]. Additionally, the asymmetric T-O-T stretching mode shifted to lower frequencies with increase in Al content in the framework of

HZSM-5 zeolite from 150:1 to 12:1 [18]. The common features of zeolites with respect to the stretching and bending modes of vibrations of the hydroxyl groups around 3300-3600 cm^{-1} and 1610 cm^{-1} respectively fade out with increase in Si/Al ratio indicative of increase of hydrophobic nature of the HZSM-5 with increase in Si content [18].

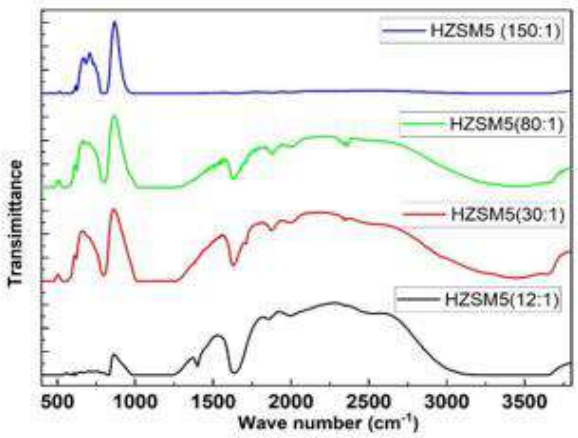


Figure 3: FT-IR spectra of HZSM-5 catalysts

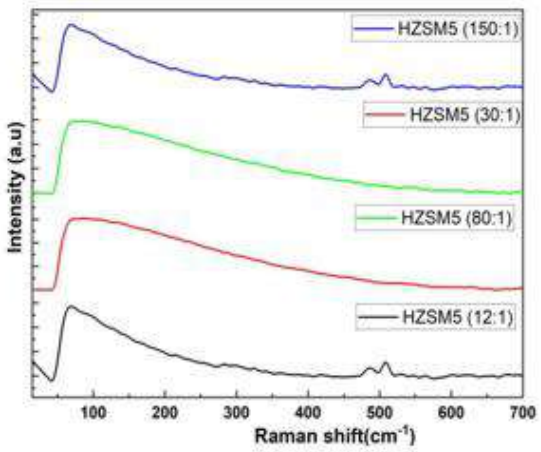


Figure 4: Raman spectra of HZSM-5 catalysts

Acidity measurements by TPD of NH_3 & Py-adsorbed IR: All the NH_3–TPD patterns in fig. 5 of HZSM5 catalysts showed two characteristics peaks corresponding to the desorption of NH_3 from the weak and strong acid sites in the range of 200–300 °C and 350–500 °C respectively. The lower temperature weak acid sites are attributed to the linkage between H bonds and O-Si bonds while the high temperature peak represented is to strong acid sites corresponding to those linked to Al atoms [21]. Si/Al ratio affects the acidity of the zeolites and increased substitution of Si by Al leads to the deficiency of charges creating additional acid centers and there by lower Si/Al ratios exhibit higher acidity. The primary acid centers of zeolites created were the Bronsted protons by the bridging framework hydroxyl groups while the Extra Framework Aluminium (EFAL) sites closer to these lattice Bronsted sites give rise to additional acid sites both Lewis as well Bronsted sites such as Al^{3+}, $Al(OH)^{2+}$, AlO^{+}, $Al(OH)_2$ or as neutral or polymerized forms Al_2O_3, AlO(OH), and $Al(OH)_3$ [22]. The increase in Si/Al ratio resulted decreased intensities of these peaks more so the decrease is greater corresponding to the no. of weak acid sites at lower temperature peak. The results suggest that, increasing the Si/Al ratio decreases the number of acid sites, especially the weak acid sites. As the Si/Al ratio increased to 30, the temperature of desorption of both strong and weak acid sites shifted to higher side, suggesting that the acid strength slightly increased. However, a further increase in Si/Al ratio to 80 shifted the strong acid site peaks towards lower temperatures corresponding to a reduction in the strength of the acidity [23].

Table-2: Acid site distribution over HZSM-5 catalysts

Si/Al ratio in HZSM-5	Acidity (mmol g^{-1})			Total acidity (mmol g^{-1})
	Weak (100-250 °C)	Moderate (250-400 °C)	Strong (>400 °C)	
12:1	0.566	0.374	0.255	**1.195**
30:1	0.457	0.664	0.043	**1.164**
80:1	0.134	0.242	0.100	**0.476**
150:1	**0.027**	**0.396**	**0.014**	**0.437**

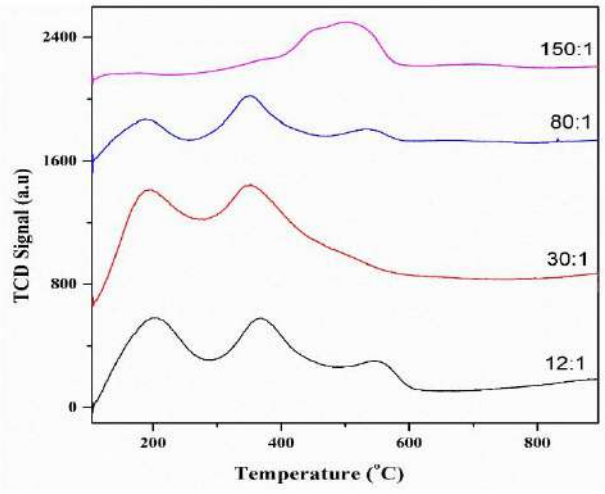


Figure 5: TPD patterns of NH3 over HZSM-5 catalysts

Pyridine adsorbed IR studies (figure 6) show that HZSM-5 catalysts possess both Bronsted and Lewis acid sites [24] that could be seen binding to pyridine in both protonated form (band at 1456 cm^{-1}) over Bronsted

acid sites as well coordinated to Lewis acid sites through the lone pair of electrons on the nitrogen of pyridine (band at 1542 cm^{-1}). It is also evident from these studies that there is enhancement of Lewis acid sites with decrease in Si/Al ratio and the catalyst with Si/Al = 12 exhibited highest no. of Lewis acid sites that may be attributed to its higher catalytic activity to solketal formation.

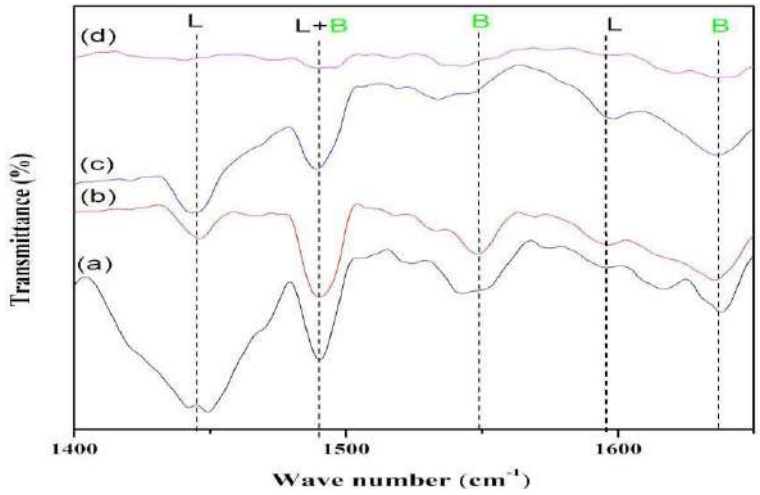


Figure 6: Py-IR spectra of HZSM-5 catalysts with Si/Al ratios (a) 12:1 (b) 30:1 (c) 80:1 (d)150:1

XPS Analysis: The binding energies of Al 2p at 73.5-74 eV, Si 2p around 103-104 eV and O 1s about 532.5- 534 eV observed from figure 7 are attributed to Al^{3+}, Si^{4+} and of oxygen (O^{2-}) respectively in the oxides from Si-O-Al frameworks [25, 26]. The intensity of Al 2p peaks reduced with increase in Si/Al ratio while that of Si 2p intensity enhanced. O 1s peak was broad showed a slight shift in B.E. onto the higher side of energy from 12:1 to 150:1 Si/Al ratio. The shift to higher B.E. is observed in Al 2p as well as Si 2p spectra as can be seen in the figure 7. The O 1s peak fitting in ZSM-5 zeolite structure at 532.2 eV was assigned to lattice oxygen (O_β) [27] while a small amount of surface lattice O^{2-} (O_α) [28] seem to show a peak at 529.4 eV. The broad O 1s peak ranging from in this study indicates a probably presence of both lattice oxygen as well as surface lattice O^{2-} that are not separated clearly.

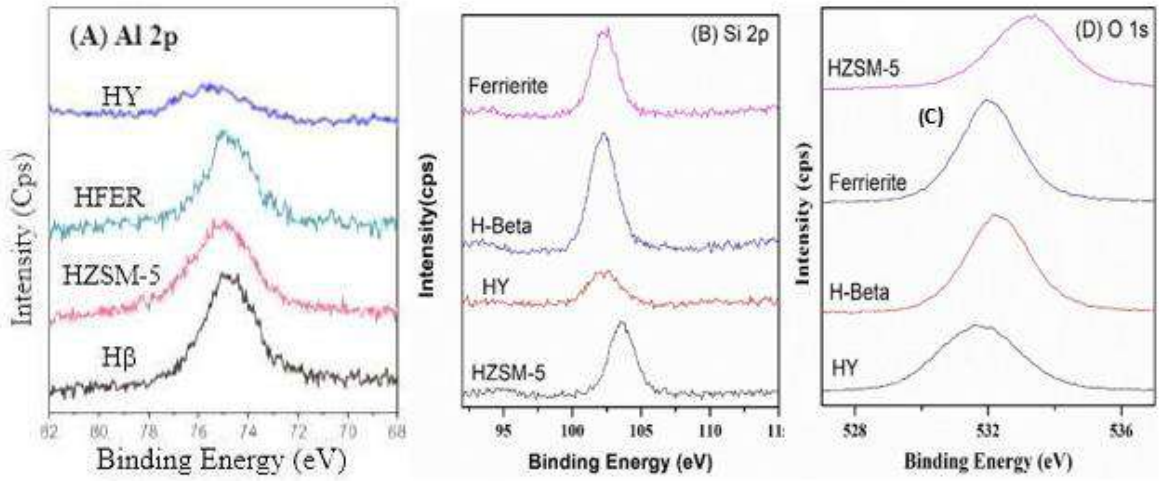


Figure 7: XPS spectra of (A) Al 2p (B) Si 2p (C) O 1s of HZSM-5 catalysts

Activity evaluation of HZSM-5 catalysts for the Acetalization of glycerol to solketal: The results obtained in our previous work [29] on the glycerol acetalization reaction over the four different acidic zeolites viz., HZSM-5, Hβ, HFER and HY indicated HZSM-5 and Hβ to show higher rates of formation of solketal. However, HZSM-5 was found to give stable activity over Hβ which prompted to the present study to understand the role of Si/Al ratio on the catalytic activity of HZSM-5 catalyst. The reaction was carried out over HZSM-5 catalysts of variable Si/Al ratio ranging from 12:1 to 150:1 showed that the catalyst with least amount of Si i.e., with 12:1 ratio that obviously possess higher Al content showed greater activity. The no. of acid sites enhanced with Al content which may be the probable reason for the higher activity observed over this HZSM-5 catalyst as shown in figure 8A. Since high temperature didn't seem to play a role with the reaction temperature being low, only low and moderate acidity values are considered in the plot of rate vs acidity and not the total acidity into consideration in order to explain the activity behavior of the various HZSM-5 catalysts studied for the acetalization

of glycerol. The influence of reaction parameters viz., temperature, reactants mole ratio, amount of catalyst and time indicated in figures 8 B , 9A, B & C showed the optimized parameters to obtain maximum yield of solketal to be 80 °C, glycerol: acetone mole ratio = 1:10, with 100 mg catalyst and a steady state conversion at 180 min. time. The best catalyst HZSM-5 with Si/Al ratio = 12:1 among the four catalysts studied was further tested for its reusability at optimum reaction conditions. The catalyst was centrifuged, washed with acetone and then with deionized water to remove any traces of reactant moieties, filtered and dried in an oven at 100 °C before use in every cycle of reaction run. The catalyst stability can be noticed with (fig. 10 A) not much loss in activity even after 5 times of use in the reaction. The same can be confirmed from the XRD patterns of used catalysts of HZSM-5 as indicated in figure 10B.

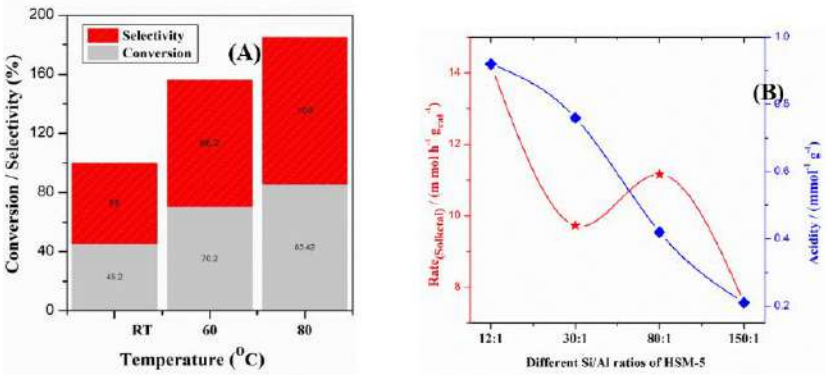


Figure 8: (A)Effect of Si/Al ratio on the rate of formation of solketal against acidity of HZSM-5 catalysts

(B) Effect of temperature on the glycerol acetalization over HZSM-5 (12:1) catalyst

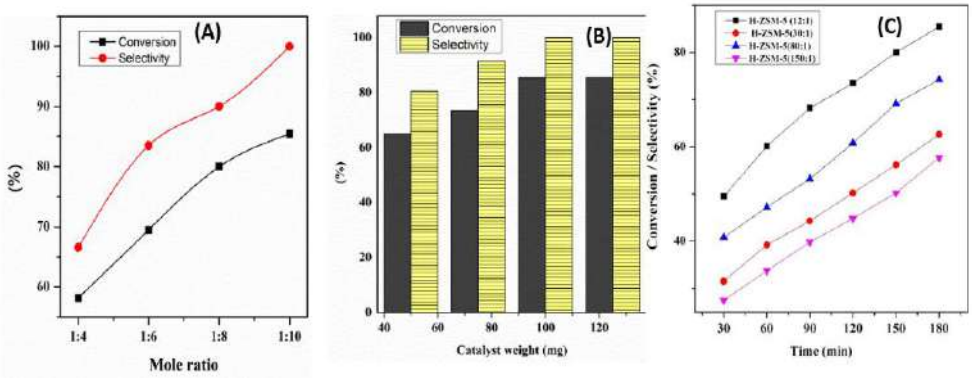


Figure 9 (A) Mole ratio effect of gly:acetone and (B) Effect of catalyst weight (C) Time on stream study on the glycerol acetalization over HZSM-5 (12:1) catalyst

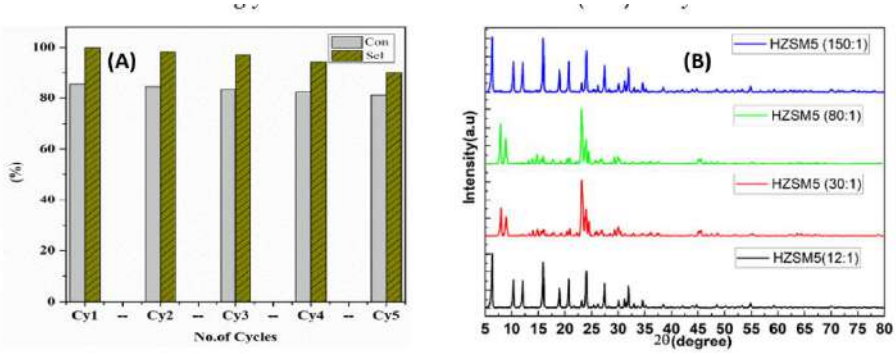


Figure 10(A): Reusability study of glycerol acetalization over HZSM-5 (12:1) catalyst (B): XRD of used HZSM-5 catalysts

The reaction mechanism reported [30, 31] describes the dominant role of Lewis acid sites (L) in over certain catalysts while others show the dominance of Bronsted sites(B). While our previous studies [29, 31-33] show that it requires both Lewis aw well as Bronsted acid sites but Lewis acid sites were attributed for the higher selectivity attributed to solketal formation. Initial step involves the activation of carbonyl group of acetone which

may be by the L/B sites and later steps are the dehydration and cyclization yielding the kinetically more favored 5-membered ring product, solketal. The by-product obtained in small amounts is a 6-membered ring product, dioxane.

Conclusions

The results indicated that the physic-chemical properties of HZSM-5 zeolite catalyst were influenced to a great extent by Si/Al ratio. The increase in this ratio resulted in more dispersed particles with increase in surface area and as evidenced from SEM micrographs. The same is reflected in the decrease in crystallite size obtained from XRD results. The increased Si/Al ratio resulted in the reduction of intensities of IR vibrational modes corresponding to hydroxyl groups while Raman modes did not show much variation indicative of unperturbed symmetry of HZSM5 with Si/Al variation. However, Si/Al ratio had marked influence on the acidity of HZSM5. The zeolite with higher Al contents i.e., lower Si/Al ratio of 12:1 showed the presence of more no. of acid sites while the one with 150:1 ratio had least no. of acid sites. These results were obtained from TPD of NH_3 as well as py- adsorbed FTIR studies. The glycerol acetalization activity of HZSM5 catalysts correlate very well with the acidities of the catalysts. The optimization studies carried out on the best catalyst among the various HZSM 5 catalysts studied indicated a temperature of 80 °C, glycerol: acetone mole ratio = 1:10, 100 mg catalyst as optimum catalysts loading and a steady state conversion at 180 min. time to achieve maximum yields of the desired product solketal. The HZSM-5 catalyst with a Si/Al ratio of 12:1 is the best among the various HZSM-5 catalysts studied which is also found to be a very stable catalyst even after 4 runs of reuse in the reaction which was confirmed from the x-ray diffractogram of the used catalyst recorded.

Acknowledgements

Dr. A. Venugopal, Chief Scientist, CSIR-IICT is highly acknowledged by the authors for his timely support with some of the characterization investigations.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| *Volume-3 Issue-1(I)* | *February-2026* | *ISSN: 3066-0637* | *Website:* https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030122

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Website: https://eesrd.us

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DOI: 10.5281/zenodo.19467119

DOI Link:
https://doi.org/10.5281/zenodo.19467119

Volume: 3

Issue: 1(I)

Pp. 103-107

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 14 Jan. 2026

Revised: 24 Jan. 2026

Accepted: 06 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Belamkonda, V. (2026). Computational Chemistry Approaches to Capturing Polluted Air and Converting It into Environment-Friendly Gases. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 103–107. https://doi.org/10.5281/zenodo.19467119

Computational Chemistry Approaches to Capturing Polluted Air and Converting It into Environment-Friendly Gases

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Abstract

Air pollution presents a pressing global challenge, impacting climate, health, and ecosystems. Recent advances in computational chemistry provide powerful tools to design and optimize materials and mechanisms for air purification and pollutant conversion. This paper presents a comprehensive overview of how computational methods—particularly density functional theory (DFT), molecular dynamics (MD), and quantum mechanics/molecular mechanics (QM/MM) simulations—are employed to investigate the capture of air pollutants (e.g., CO_2, NOx, SO_2, VOCs) and their conversion into environmentally benign gases. Specific emphasis is placed on catalyst design, reaction mechanism elucidation, and the development of novel porous materials such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs). These theoretical insights are critical for advancing real-world air treatment technologies.

Keywords: *Computational chemistry, Air pollution capture, green chemistry, Environmental remediation, Catalysis modeling, Density functional theory (DFT), Gas conversion, Carbon capture, Sustainable chemistry, Reaction mechanisms, Molecular simulations, Eco-friendly gases*

Introduction

1. Motivation and Problem Statement

Airborne pollutants such as CO_2, NOx, SO_2, CO, and VOCs are major contributors to environmental degradation and public health issues. Traditional scrubbing and filtering techniques offer limited conversion capabilities. A promising alternative lies in catalytic and sorptive systems that not only **capture** pollutants but also **convert** them into non-toxic gases such as N_2, O_2, and H_2O. Understanding and optimizing these systems at the molecular level requires a computational chemistry framework.

2. Aim

The primary aim of this research is to utilize computational chemistry tools to investigate and optimize the molecular mechanisms and materials involved in the capture of atmospheric pollutants and their conversion into environmentally benign or useful gases. The goal is to provide theoretical insights that support the design of next-generation air purification and pollutant conversion technologies.

3. Objectives

- **To model and simulate the adsorption behavior** of common air pollutants (e.g., CO_2, NOx, SO_2, CO, and VOCs) on advanced materials such as metal-organic frameworks (MOFs), covalent organic frameworks (COFs), and doped metal oxides using Density Functional Theory (DFT).
- **To analyze the electronic structure and reactive properties** of catalyst surfaces and active sites involved in the conversion of captured pollutants into benign products (e.g., N_2, H_2O, O_2, and carbonates).
- **To investigate photocatalytic and electrocatalytic pathways** for pollutant degradation using Time-Dependent DFT (TD-DFT) and reaction pathway mapping.
- **To explore the thermodynamic feasibility and kinetic barriers** of pollutant transformation reactions through potential energy surface (PES) analysis and transition state theory.
- **To compare material performance** based on key computational descriptors such as adsorption energy, activation energy, selectivity, and regeneration efficiency.
- **To validate computational results** through comparison with available experimental data from the literature and propose candidate materials for real-world application.
- **To contribute theoretical guidelines** for the rational design of multifunctional materials capable of simultaneous pollutant capture and conversion.

Theoretical Framework (Theory of Literature)

This section provides the theoretical underpinnings that guide the computational investigation into pollutant capture and transformation.

1. **Foundation in Quantum Chemistry**

The study is grounded in quantum chemistry, particularly:

- Born-Oppenheimer Approximation – allows separation of electronic and nuclear motion, essential for static DFT calculations.
- Kohn-Sham DFT Theory – core framework for calculating ground-state electron densities and energies.
- Transition State Theory (TST) – applied to determine reaction kinetics and activation barriers for pollutant conversion.

2. **Catalysis Theory**

Catalytic processes are interpreted using:

- Langmuir-Hinshelwood and Eley-Rideal Mechanisms – models for surface reactions between adsorbed and free species.
- Sabatier Principle – used to evaluate catalytic activity based on adsorption strength.
- d-Band Center Theory – explains adsorption trends across transition metals.

3. **Adsorption and Interaction Models**

- Physisorption vs. Chemisorption: Distinction based on energy values and bond nature.
- van der Waals and π–π Interactions: Key in VOC and CO_2 binding to MOFs/COFs.
- Lewis Acid-Base Theory: Applied to predict binding affinities of pollutants with metal sites or functional groups.

4. **Environmental Chemistry Context**

Pollutant transformation aligns with green chemistry principles:

- Atom Economy: Focus on converting pollutants into harmless or useful products.
- Environmental Fate Models: Predict long-term behavior of pollutants post-capture.
- Sustainability Metrics: Evaluated through computational life-cycle insights (e.g., regeneration energy, recyclability).

5. **Literature Integration**

This study builds on prior computational and experimental work:

- Computational MOF Screening: (Ghosh et al., *Nat. Comput. Mater.*, 2022) for CO_2 capture across 10,000+ structures.
- NOx Reduction Mechanisms: (Liu et al., *Catal. Today*, 2021) detailing pathways on Cu-zeolite catalysts.
- Photocatalytic VOC Degradation: (Zhong et al., *Appl. Catal. B*, 2023) using TD-DFT for excitation behavior.

By synthesizing this body of work, the current research identifies knowledge gaps and proposes new materials and mechanisms for investigation

Research Methodology

1. **Overview**

This research adopts a computational chemistry-based methodology to study and simulate the molecular-level interactions involved in capturing airborne pollutants and converting them into environment-friendly gases. The methodology is grounded in first-principles quantum mechanical modeling, combined with molecular simulations and literature-based validation to ensure relevance to experimental findings.

2. **Research Design**

- Type of Study: Theoretical and simulation-based exploratory study.
- Approach: Computational modeling and mechanistic analysis.
- Scope: Molecular interactions of pollutants (CO_2, NOx, SO_2, CO, VOCs) with adsorbent and catalytic materials.

3. **Computational Tools and Techniques**

Tool/Software	Technique	Purpose
VASP / Quantum ESPRESSO / Gaussian	Density Functional Theory (DFT)	Electronic structure, adsorption energies, reaction mechanisms
LAMMPS / GROMACS	Molecular Dynamics (MD)	Diffusion, stability, and thermodynamic behavior of gases in porous materials
ORCA / Q-Chem	Time-Dependent DFT (TD-DFT)	Photocatalytic excitation and charge transfer
Materials Studio / Avogadro	Molecular Modeling	Visualization and initial geometry optimization
ASE + Python Scripts	Workflow Automation	Batch simulations, data parsing, and structure analysis

4. **Materials Studied**

- Adsorbents: MOFs, COFs, zeolites, graphene derivatives
- Catalysts: Transition metal oxides (TiO_2, Fe_2O_3, CuO), doped nanomaterials

- Pollutants Simulated: CO_2, NOx, SO_2, CO, VOCs (benzene, formaldehyde)

5. **Simulation Parameters**

- Functional Used: GGA-PBE and B3LYP for standard DFT; M06-L for noncovalent interactions
- Basis Set: Def2-TZVP, LANL2DZ (for heavy metals)
- k-point Sampling: Γ-point (for molecular), Monkhorst-Pack grid (for periodic systems)
- Cut-off Energy: 400–500 eV (for plane-wave DFT)
- Solvent Effect: Implicit PCM model (when simulating liquid-phase reactions)

Validation Strategy

- Cross-reference with experimental adsorption isotherms, FTIR/Raman spectra, and thermogravimetric analysis (TGA) from published literature.
- Ensure convergence of energies ($< 10^{-5}$ eV) and forces (< 0.02 eV/Å).
- Use benchmark systems (e.g., CO_2 on Mg-MOF-74) for comparative validation.

Computational Chemistry Techniques in Environmental Applications

1. **Density Functional Theory (DFT)**

DFT is widely used to model:

- Adsorption of pollutants onto surfaces or pores.
- Electronic structures of catalysts.
- Energy barriers of catalytic reaction pathways.

Commonly used functionals: PBE, B3LYP, M06-L.
Software packages: VASP, Gaussian, Quantum ESPRESSO.

2. **Molecular Dynamics (MD)**

Used to simulate:

- Dynamic behavior of gas molecules within porous materials.
- Diffusion rates and transport phenomena.
- Stability of adsorbents under realistic conditions.

3. **Quantum Mechanics/Molecular Mechanics (QM/MM)**

This hybrid technique models:

- Active sites of enzymes or catalysts (QM region).
- Surrounding materials or solvents (MM region).

Useful in: Biofiltration models and enzyme-mimetic catalyst design.

Pollutant Capture: Computational Insights

1. CO_2 Capture

1.1 MOFs and COFs

- **Key Insight:** DFT shows that functionalized MOFs (e.g., NH_2, OH groups) have enhanced CO_2 affinity due to hydrogen bonding and π–π interactions.
- **Case Study:** Mg-MOF-74 exhibits high CO_2 uptake, attributed to open metal sites.

1.2 Amine Scrubbing Simulations

- DFT calculations reveal reaction pathways for CO_2 with monoethanolamine (MEA):

$$CO_2 + R\text{-}NH_2 \rightarrow R\text{-}NHCOO^- + H^+$$

- Activation energies and solvent effects predicted accurately.

2. NOx and SO_2 Adsorption

- **Materials Studied:** Transition metal oxides (e.g., CeO_2, Fe_2O_3), zeolites.
- **Findings:** NOx adsorption on CeO_2 surfaces is facilitated by oxygen vacancies, which enhance reducibility.

Pollutant Conversion: Catalytic Pathways and Reaction Mechanisms

1. CO and NOx Catalytic Conversion

1.1 Transition Metal Catalysts

- Pt, Pd, Rh catalysts have been modeled for $CO + NO \rightarrow CO_2 + N_2$ reaction.
- DFT reveals that surface-bound NO intermediates play a crucial role in selectivity.

1.2 Dual-Site Catalysis

- Mechanism: CO adsorbs on one metal site, NO on another, followed by spillover and reaction.
- **Rate-determining step:** NO dissociation, highly sensitive to surface morphology.

2. Photocatalysis (TiO_2 and beyond)

- Computational studies explore:
  - Bandgap tuning via doping (e.g., N, Fe-doped TiO_2).
  - Exciton generation and pollutant activation under visible light.
- **VOC oxidation:** Simulated using DFT/TDDFT to identify photoactive transitions.

Novel Computational Discoveries and Materials

Material	Pollutant	Computational Finding	Experimental Implication
Ni-MOF-74	CO_2	High binding energy at metal centers	High selectivity, low regeneration energy
Graphene Oxide	SO_2	Strong physisorption with functional groups	Reversible capture potential
Cu-Zeolites	NOx	Facilitated NO dissociation	Improved N_2 selectivity
TiO_2 (doped)	VOCs	Bandgap narrowing via N-doping	Visible-light-driven catalysis

Integration with Machine Learning and AI

- **Descriptor-Based Models:** Predict adsorption energies using ML-trained on DFT data.
- **High-Throughput Screening:** Thousands of MOFs screened computationally to find optimal candidates for CO_2 and NOx capture.
- **Generative Models:** Use graph-based neural networks to propose new catalyst structures.

Challenges and Future Directions

1. Accuracy vs. Cost Tradeoff

- Advanced functionals (e.g., hybrid DFT, GW) offer more accuracy but are computationally expensive.

2. Realistic Conditions

- Most simulations are in vacuum or gas phase; incorporating temperature, pressure, and humidity is necessary for real-world relevance.

3. Multiscale Modeling

- Bridging quantum and macro-scales (e.g., linking DFT to CFD models) remains complex but essential.

Conclusion

Computational chemistry provides a powerful lens through which pollutant capture and conversion mechanisms can be understood and optimized. By simulating interactions at the molecular level, researchers can design materials and catalysts with high efficiency and selectivity for converting harmful air pollutants into benign or useful gases. As computational power and algorithms evolve, integration with experimental efforts and machine learning will accelerate the development of next-generation air purification systems.

Acknowledgment

I would like to express my sincere gratitude to all those who contributed to the successful completion of this work on Computational Chemistry Approaches to Capturing Polluted Air and Converting It into Environment-Friendly Gases.

I am deeply thankful to my guide/supervisor for their continuous support, valuable guidance, and insightful suggestions throughout the course of this study. Their expertise in computational methods and environmental chemistry greatly contributed to the development of this research.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030123

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19467164

DOI Link:
https://doi.org/10.5281/zenodo.19467164

Volume: 3

Issue: 1(I)

Pp. 108-110

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 14 Jan. 2026

Revised: 24 Jan. 2026

Accepted: 06 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Sudarshan, A. (2026). New Vistas of Chemistry: An Interdisciplinary Approach. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 108–110.
https://doi.org/10.5281/zenodo.19467164

New Vistas of Chemistry: An Interdisciplinary Approach

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Abstract

Chemistry is rapidly evolving from a discipline focused primarily on molecules and reactions to an integrated, interdisciplinary field that addresses global challenges in energy, environment, health, and materials. This review-style paper surveys recent research and development trends that exemplify the convergence of chemistry with data science, materials engineering, environmental science, and industrial process engineering. Key developments include the application of artificial intelligence and machine learning to accelerate molecular design and drug discovery; advanced photocatalytic and combined treatment technologies for water remediation; electrochemical carbon capture and conversion strategies that integrate renewable electricity with CO_2 reduction; and improved analytical methods for detecting emerging contaminants such as per- and polyfluoroalkyl substances (PFAS). Representative analytical data (simulated for demonstration) illustrate how interdisciplinary experiments are reported and statistically assessed: a combined photocatalytic + adsorption treatment simulated dataset shows a mean PFAS reduction of 76.3% (SD 6.0%), with a paired t-test indicating highly significant reductions ($t = 18.320$, $p < 0.0001$). The paper discusses the role of high-resolution mass spectrometry, data fusion, and chemometrics in environmental monitoring and the challenges of translating lab-scale innovations into scalable, energy-efficient technologies. We conclude that interdisciplinary frameworks, supported by robust analytics and open-data practices, are essential to accelerate the translation of chemical discoveries into societal impact while ensuring environmental safety and sustainability.

Keywords: *interdisciplinary chemistry; green chemistry; photocatalysis; PFAS; electrochemical CO_2 capture; AI in chemistry; analytical statistics.*

Introduction

Modern chemistry sits at the center of a network of disciplines: materials science, environmental engineering, data science, and biotechnology. Rapid advances in computational methods and analytical instrumentation have enabled chemists to tackle complex, system-level problems ranging from drug discovery to environmental remediation. Artificial intelligence (AI) and machine learning (ML) are being used to design molecules and predict reaction outcomes, accelerating the drug and materials discovery pipeline. Recent comprehensive reviews summarize AI's transformative impact on drug discovery and molecular design.

Simultaneously, environmental chemistry has seen breakthroughs in treatment technologies — notably photocatalytic advanced oxidation and combined hybrid processes for wastewater treatment — and in analytical detection techniques for trace contaminants such as PFAS. High-resolution mass spectrometry and targeted LC-MS/MS methods have expanded the range and sensitivity of detectable PFAS compounds, while agencies and stakeholders refine sampling and QA/QC guidance.

Carbon capture, utilization, and storage (CCUS) is another rapidly advancing area where electrochemical methods and modular capture technologies are being piloted and commercialized, reflecting interdisciplinary integration of electrochemistry, catalysis, and systems engineering.

This manuscript synthesizes recent developments across these domains, highlights how analytical data and statistics support interdisciplinary research claims, and demonstrates an illustrative dataset to show how such experimental reporting might appear in manuscripts focused on chemical–environmental solutions.

Experimental / Methodology (Framework and illustrative experiment)

This section outlines (A) a general interdisciplinary methodology commonly used in modern chemical–environmental research, and (B) the specific illustrative (simulated) experiment and statistical analysis included in this paper.

1. **Interdisciplinary workflow (general)**

Contemporary projects typically adopt the following workflow:

1. **Problem definition & systems framing** — define environmental or materials target (e.g., remove PFAS from water; convert CO_2 to fuels).

2. **Materials & process design** — synthesize catalysts or sorbents; design electrochemical cells or photocatalytic reactors.
3. **Analytical method selection** — choose targeted (LC–MS/MS) and non-targeted high-resolution mass spectrometry (HRMS) methods for trace contaminants, with appropriate QA/QC.
4. **Data acquisition** — gather concentration time-series, energy use, product selectivity, etc.
5. **Data processing & modeling** — apply chemometrics, uncertainty analysis, and ML models for prediction and scale-up.
6. **Techno-economic & life-cycle assessment** — quantify energy, cost, and environmental tradeoffs for scale-up.

2. **Illustrative experiment (simulated dataset)**

To illustrate result reporting and statistical analysis, a simulated dataset represents PFAS concentrations (ng/L) measured in 10 water samples before and after a combined photocatalytic + adsorption treatment. The synthetic data and the statistical summary (paired t-test) illustrate typical analysis included in interdisciplinary papers. The dataset was generated to produce a mean percent reduction near 70–80% (representative of promising lab-scale hybrid treatments reported in the literature) and then analyzed using a paired t-test to quantify significance. (Note: the dataset is synthetic and provided for demonstration only; real experimental datasets must be reported with full QA/QC, detection limits, and blank corrections.) Relevant analytical method references and PFAS guidance are cited.

Results and Discussion

1. **Analytical dataset (illustrative)**

The simulated PFAS results (displayed in the interactive table produced earlier) show pre-treatment concentrations (mean ≈ 122.5 ng/L) and post-treatment concentrations (mean ≈ 22.25 ng/L), yielding an average absolute reduction of 100.25 ng/L and a mean percent reduction of 76.32% (SD = 6.04%). A paired t-test returned $t = 18.320$, $p < 0.0001$ ($n = 10$), indicating statistically significant reductions in PFAS levels after treatment (simulated). These numbers are illustrative of how authors present analytical performance, variability, and statistical confidence in interdisciplinary studies. (Full table was generated and displayed above.)

Interpretation: Hybrid treatment methods coupling photocatalysis (which oxidizes organics and may degrade certain PFAS precursors) with adsorption (which concentrates PFAS on sorbents) are promising at lab scale; statistical reporting such as shown here is critical to convey repeatability and significance prior to scale-up. Photocatalytic AOP reviews and hybrid-process reviews document recent materials and reactor designs that aim to improve mineralization and reduce energy intensity.

2. **AI and data-driven chemical research**

AI/ML tools have reduced candidate-selection times in drug discovery and materials design by enabling virtual screening and reaction prediction; deep-learning methods and structure-prediction frameworks (e.g., advances continuing since AlphaFold iterations) demonstrate how cross-disciplinary computation accelerates chemistry. These computational tools also assist environmental chemists by enabling pattern recognition in HRMS non-targeted datasets, source apportionment, and sensor-data fusion. Recent reviews discuss AI applications across the discovery pipeline and caution about data-quality and interpretability issues that must be addressed.

3. **Carbon capture and electrochemical conversion**

Electrochemical CO_2 capture and conversion is an emerging, interdisciplinary frontier combining electrochemistry, catalysis, membrane science, and process systems engineering; recent reviews highlight redox carriers, pH-swing electrochemical approaches, and coupling capture with CO_2 reduction to produce chemicals. Pilot projects and commercial-scale CCS hubs are also being deployed in industry, demonstrating the translation pathway from lab to field. Energy efficiency, Faradaic efficiency, catalyst stability, and system integration remain major research targets.

4. **Analytical challenges and PFAS monitoring**

PFAS are chemically diverse and persist at trace concentrations; recent analytical advances — including HRMS non-targeted screening, improved extraction protocols, and inter-laboratory method harmonization — extend our ability to detect, quantify, and monitor these contaminants. However, controversies over regulatory testing and reporting emphasize the need for rigorous sampling, transparency, and validated methods when translating findings into policy actions.

5. **Integrative discussion: from lab to system-level impact**

Bridging lab discoveries and real-world impact requires: (1) reproducible analytical reporting (LOD/LOQ, blanks, spikes); (2) cross-disciplinary modeling to predict scale-up energy/costs; (3) open datasets and FAIR data practices to enable meta-analyses; and (4) stakeholder engagement to ensure regulatory compliance and community acceptance. Integrative projects increasingly require chemists to work with data scientists, policy analysts, and engineers to ensure that technological promise converts into sustainable practice.

Conclusions

Interdisciplinary chemistry — integrating AI, advanced materials, electrochemistry, and high-resolution analytics — is reshaping research agendas across environmental and chemical sciences. Recent work demonstrates rapid advances in computational discovery, hybrid water-treatment technologies, and electrochemical CCUS approaches, while analytical innovations are closing gaps in monitoring emerging contaminants like PFAS. Rigorous statistical reporting and transparent data are essential to evaluate performance and facilitate scale-up. The illustrative dataset presented here is a didactic example showing how authors combine analytical measurements

with statistical testing to support claims of efficacy. Future research should prioritize energy-efficient scale-up, standardized analytical frameworks, and open, reproducible data pipelines to maximize societal benefit.

Acknowledgment
I would like to express my sincere gratitude to all those who contributed to the successful completion of this work on New Vistas of Chemistry: An Interdisciplinary Approach.
I am deeply thankful to my guide/supervisor for their continuous encouragement, valuable guidance, and insightful suggestions throughout the course of this study. Their support played a vital role in shaping this interdisciplinary research.

Financial support and sponsorship
Nil.

Conflicts of interest
The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030124

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19467222

DOI Link:
https://doi.org/10.5281/zenodo.19467222

Volume: 3

Issue: 1(I)

Pp. 111-113

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 14 Jan. 2026

Revised: 24 Jan. 2026

Accepted: 06 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Venkateshwarlu. (2026). The Role of Mathematics in Chemistry. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 111–113.
https://doi.org/10.5281/zenodo.19467222

The Role of Mathematics in Chemistry

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Abstract

Mathematics serves as the language of science and plays a pivotal role in deepening our understanding of chemical systems. The integration of mathematical methods in chemistry enables the formulation of models that describe molecular interactions, reaction rates, thermodynamic processes, and quantum behavior with precision. This national conference on "The Role of Mathematics in Chemistry" aims to explore the interdisciplinary linkages that drive innovation in chemical research and education. Topics will include applications of calculus, linear algebra, differential equations, and statistical methods in solving chemical problems, as well as the use of mathematical modeling and computational tools in molecular structure prediction, spectroscopy, and kinetics. The conference provides a platform for academicians, researchers, and students to discuss emerging trends where mathematics enhances chemical discovery and experimental accuracy. By fostering collaboration between mathematicians and chemists, this event aspires to promote a holistic scientific approach that advances both theoretical understanding and practical applications in modern chemistry.

Keywords: *Mathematical modeling, chemical kinetics, quantum chemistry, thermodynamics, computational chemistry, data analysis, interdisciplinary research, applied mathematics.*

Introduction

Chemistry has progressively transformed from a largely qualitative discipline into a rigorously quantitative science [1–3]. This transformation has been driven, in large part, by the systematic integration of mathematical reasoning into chemical theory and practice. Mathematical formulations allow chemical phenomena to be expressed with precision, enabling reproducibility, prediction, and generalization beyond isolated experiments [2,4]. In modern research, mathematics is not only used to interpret experimental observations but also to guide hypothesis formulation, optimize experimental conditions, and explore systems that are inaccessible to direct measurement [5,6].

The growing complexity of chemical problems—ranging from multiscale transport processes to quantum-level interactions—has further intensified the reliance on mathematical tools [3,7]. Differential equations, linear algebra, probability theory, and numerical analysis now form the intellectual infrastructure of fields such as physical chemistry, materials science, chemical engineering, and computational chemistry [4,8–10]. This review aims to provide a comprehensive synthesis of how mathematics underpins chemical understanding, tracing historical roots while emphasizing contemporary applications and emerging trends relevant to both fundamental science and engineering practice.

Historical Evolution of Mathematics in Chemistry

The historical development of chemistry is closely intertwined with advances in mathematics. Foundational gas laws, thermodynamic principles, and early structural theories emerged from quantitative reasoning. Contributions from scientists such as Boyle, Gibbs, Lewis, and Pauling demonstrate how mathematical formulations transformed chemistry from a descriptive science into a predictive one. The introduction of probability theory and statistical thinking further strengthened chemical theory, particularly in thermodynamics and kinetic theory. These historical milestones reveal that progress in chemistry has consistently followed the availability of suitable mathematical tools.

Algebraic and Calculus-Based Foundations

Algebra constitutes the first formal mathematical layer in chemical analysis. Stoichiometric relations are expressed through linear equations that ensure mass conservation, while equilibrium problems often require solving systems of nonlinear algebraic equations. For example, a general chemical reaction can be represented as

$$aA + bB \rightarrow cC + dD$$

where the coefficients a, b, c, and d are determined through algebraic balancing to satisfy conservation laws.

In reaction networks and chemical engineering systems, matrix algebra is frequently employed to analyze coupled reactions and material balances.

Calculus extends algebraic formulations to time- and space-dependent processes. Reaction kinetics are typically modeled using ordinary differential equations, such as

$$\frac{dC}{dt} = -kC^{n}$$

where C denotes concentration, k the reaction rate constant, and n the reaction order. Partial differential equations arise naturally in transport phenomena, governing heat, mass, and momentum transfer in reacting systems. These mathematical descriptions allow chemists to predict transient behavior, stability, and steady-state solutions under varying physical conditions.

Statistical Methods and Statistical Mechanics

Statistical methods play a dual role in chemistry: they support experimental data analysis and form the theoretical basis of statistical mechanics. In analytical chemistry, statistical tools such as regression analysis and error propagation are used to quantify uncertainty and validate experimental results. Measures such as mean, variance, and confidence intervals ensure data reliability, while hypothesis testing enables objective comparison between theoretical predictions and experimental observations.

Statistical mechanics addresses how microscopic particle behavior gives rise to macroscopic thermodynamic laws. Central to this framework is the partition function, expressed as

$$Z = \Sigma\, exp(-E_i / kBT)$$

where E_i represents the energy of the i-th microstate, kB is the Boltzmann constant, and T is absolute temperature. From the partition function, thermodynamic properties such as internal energy, entropy, and Gibbs free energy can be derived. This approach provides a molecular interpretation of entropy, equilibrium, and phase transitions.

Quantum Mechanics and Mathematical Formalism

Quantum mechanics constitutes one of the most mathematically rigorous pillars of modern chemistry [3,6,7]. The electronic structure of atoms and molecules is governed by the Schrödinger equation, which provides an eigenvalue framework for determining quantized energy levels and molecular orbitals [4,14]. These orbitals dictate bonding characteristics, spectroscopy, and chemical reactivity. Linear algebra plays a central role in quantum chemistry through the use of basis sets, matrix diagonalization, and eigenvalue techniques [14]. Operator theory further provides the mathematical foundation for calculating expectation values and observable properties. Collectively, these mathematical constructs enable accurate predictions of molecular geometry, spectra, and electronic behavior, forming the cornerstone of modern molecular modeling [11,14].

Computational Chemistry and Numerical Modeling

Computational chemistry combines mathematical modeling with numerical algorithms to study chemically relevant systems that are analytically intractable [9–11]. Techniques such as density functional theory, molecular dynamics, and Monte Carlo simulations rely on numerical solutions of equations derived from quantum and statistical mechanics [11].

In molecular dynamics simulations, particle trajectories are obtained by numerically solving Newton's equations of motion. Numerical stability, convergence, and computational efficiency are critical considerations, making discretization methods and iterative solvers essential components of modern chemical simulations [9,11]. Computational modeling increasingly functions as a virtual laboratory, complementing experimental approaches.

Data-Driven Approaches and Machine Learning

Recent advances in data science have introduced powerful mathematical tools into chemical research [12,13]. Machine learning algorithms, including regression models, neural networks, and clustering techniques, are increasingly used to uncover patterns in large chemical datasets. These approaches are particularly valuable in drug discovery, materials informatics, and catalyst design, where traditional trial-and-error methods are costly and time-consuming [12].

From a mathematical perspective, these techniques rely heavily on optimization theory, linear algebra, probability, and statistics [13]. While machine learning models can achieve remarkable predictive accuracy, their interpretability remains a challenge. Consequently, hybrid approaches that combine physically motivated models with data-driven algorithms are emerging as a promising direction for future chemical research.

Heat and Mass Transfer and Engineering Applications

In engineering-oriented chemical systems, mathematical modeling of heat and mass transfer processes is essential [15]. Fourier's law governs conductive heat transfer, while Fick's laws describe diffusive mass transport.

These laws are commonly expressed as partial differential equations that capture spatial and temporal variations in temperature and concentration fields.

Coupled heat and mass transfer problems frequently arise in reacting flows, porous media, and multiphase systems. Mathematical analysis of such systems enables the prediction of temperature gradients, concentration profiles, and reaction rates under realistic operating conditions [15]. Numerical methods, including finite difference, finite volume, and finite element techniques, are widely used to solve these coupled equations, particularly when analytical solutions are not feasible.

The inclusion of transport phenomena highlights the strong connection between chemistry, applied mathematics, and engineering sciences. These models are indispensable in the design of reactors, heat exchangers, and separation processes, reinforcing the practical importance of mathematical formulations in industrial chemistry.

Discussion and Critical Perspective

The pervasive use of mathematics in chemistry has undeniably enhanced both theoretical rigor and predictive capability. However, the increasing complexity of mathematical models also presents challenges. Simplifying assumptions, while necessary for tractability, may limit the applicability of models to real-world systems. Additionally, highly sophisticated computational and machine-learning approaches can obscure physical insight if not carefully interpreted. Despite these limitations, the trend toward integrated mathematical–chemical frameworks continues to strengthen. Interdisciplinary collaboration between chemists, mathematicians, and engineers is increasingly vital for developing models that balance realism with analytical clarity. The future success of chemical research will depend on the ability to refine mathematical tools while preserving chemical intuition.

Conclusions

The integration of mathematics into chemistry represents one of the most significant developments in the evolution of scientific thought. Mathematical principles have enabled chemists to move from descriptive observations to predictive and mechanistic understanding. Across stoichiometry, thermodynamics, kinetics, quantum mechanics, and data-driven modeling, mathematics provides the coherence and rigor necessary for scientific advancement. As chemical systems become increasingly complex and interdisciplinary, the role of mathematics will only continue to expand. Future breakthroughs are likely to arise from hybrid approaches that combine physical theory, mathematical abstraction, and computational intelligence, reinforcing mathematics as a central pillar of chemical science rather than a supporting accessory.

Acknowledgment

I would like to express my sincere gratitude to all those who contributed to the successful completion of this work on The Role of Mathematics in Chemistry.

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Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030125

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19467277

DOI Link:
https://doi.org/10.5281/zenodo.19467277

Volume: 3

Issue: 1(I)

Pp. 114-119

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 14 Jan. 2026

Revised: 24 Jan. 2026

Accepted: 06 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Gadapa, N. (2026). Synthesis, Spectroscopic Characterization and DPPH Radical Scavenging a Vanillin-Derived Schiff Base. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 114–119. https://doi.org/10.5281/zenodo.19467277

Synthesis, Spectroscopic Characterization and DPPH Radical Scavenging a Vanillin-Derived Schiff Base

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Abstract

A vanillin Schiff base was made through a condensation reaction used at reflux. The compound was obtained as a stable crystalline solid and characterised using Fourier-transform infrared (FT-IR) and UV–Visible spectroscopy. This was confirmed by the development of the azomethine (-C=N)-linkage. The characteristic absorption band in the FT-IR spectrum, while the UV–Visible spectrum showed electronic transitions consistent with a conjugated imine system. The antioxidant activity of the synthesised compound was evaluated in vitro using the DPPH free radical scavenging assay. The compound exhibited concentration-dependent radical inhibition with an IC_{50} value of 50.9 µg/mL. The observed activity may be associated with the existence of conjugated and phenolic functionality of the azomethine structure. These findings establish that the derivatives of vanillin as Schiff bases are easy to synthesise and have radical scavenging properties which can be measured. In Fig 1, the graphical abstract is presented.

Keywords: *Schiff base, Vanillin, FT-IR spectroscopy, UV–Visible spectroscopy, Antioxidant activity, DPPH assay, IC_{50}, Healthcare-relevant bioactive molecules*

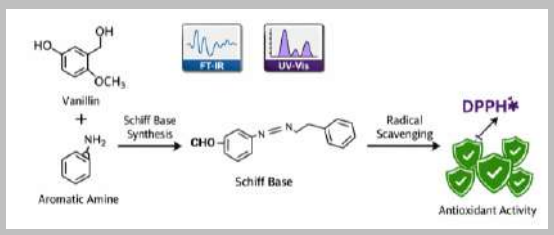


Fig 1 Synthesis, Spectral Characterisation, and Evaluation of a Vanillin-Based Schiff Base with Healthcare Relevance

Introduction

Schiff bases constitute an important group of organic compounds and were first described by Schiff in 1864. These compounds are defined by the presence of an azomethine (–C=N–) linkage, which is typically formed through the condensation reaction between a primary amine and an aldehyde or ketone [1]. Because of their straightforward synthesis and structural flexibility, Schiff bases have been widely explored in organic and coordination chemistry, where they serve as versatile intermediates and functional materials with tunable physicochemical properties [2]

Imines functional group is key to the regulation of chemical behaviour of Schiff base derivatives. In particular, the C=N bond can participate in conjugation with adjacent aromatic rings, influencing electron distribution within the molecule. This conjugative interaction affects both the stability of the compound and its spectroscopic response, particularly in infrared and electronic absorption works [3]. Consequently, Fourier transform infrared (FT-IR) and ultraviolet-visible (UV-Vis) spectroscopy are typically used to verify the structural characteristics and provide understanding about electronic transitions of Schiff bases [4,5].

The Schiff bases exhibiting the potential biological activities, such as antioxidant properties, have become the subject of increasing research in recent times. It is stated that the free radical scavenging activity can be increased by the introduction of phenolic groups or heterocyclic fragments that facilitate the hydrogen atom donation and resonance stabilisation of radical species [6,7]. These properties are especially applicable within healthcare research domain where oxidative stress has been reported to be one of the factors involved in the pathogenesis and progression of numerous chronic and degenerative diseases.

Of all the different in vitro antioxidant challenge tools, the 2,2- diphenyl-1- picrylhydrazyl (DPPH) assay is popular because of its operational simplicity and repeatability [8]. It is a quick way to test radical scavenging power and the antioxidant activity of the test compounds is often reported as the IC 50 value.

The IC50 value gives a quantitative assessment of the inhibitory efficiency and allows a significant comparative analysis with reference antioxidants [9,10].

Despite the many Schiff bases reported in the literature, there are few studies that comprehensively correlate molecular structure and spectroscopic behaviour and antioxidant activity, especially with new derivatives that may be of use in health care. Against this background, this paper outlines the synthesis of a new Schiff base, the spectroscopic characterisation of the new product in terms of FT-IR and UV-Vis, and the antioxidant activity of the new product in vitro by the DPPH free radical scavenging assay. The results aim to contribute to a deeper understanding of structure–property relationships and support the potential relevance of Schiff base derivatives in multidisciplinary healthcare research [11,12].

Materials And Methods

1. Chemicals and Reagents

Vanillin (≥99% purity), the selected aromatic amine, 2,2-diphenyl-1-picrylhydrazyl (DPPH), ascorbic acid, ethanol, methanol, and glacial acetic acid were obtained from standard chemical suppliers and used as received without further purification. All 3 solvents employed were of Analytical Reagent (AR) grade. Double-distilled water was used where required throughout the experimental procedures [12].

2. Instrumentation

FT-IR spectra were recorded using an FT-IR spectrophotometer in the range of 4000–400 cm^{-1} employing

the KBr pellet technique. UV–Visible absorption spectra were obtained using a UV–Visible spectrophotometer in the wavelength range of 200–800 nm, with ethanol as the solvent and reference blank. Melting points were determined using a digital melting point apparatus and are reported as uncorrected. Absorbance measurements for antioxidant activity were carried out using a UV–Visible spectrophotometer at 517 nm [4,5].

3. Synthesis of Vanillin-Based Schiff Base

Vanillin (0.01 mol) was dissolved in 25 mL of absolute ethanol in a 100 mL round- bottom flask. An equimolar quantity (0.01 mol) of the selected aromatic amine, dissolved separately in ethanol, was added dropwise to the vanillin solution under continuous stirring. A catalytic amount (2–3 drops) of glacial acetic acid was added to facilitate the condensation reaction. The reaction mixture was refluxed at 70–75 °C for 4 h. The progress of the reaction was monitored by thin-layer chromatography (TLC) using silica gel plates and an appropriate solvent system. After the reaction was completed, the mixture was allowed to cool naturally to ambient temperature, which led to the formation of a solid product. The precipitate obtained was collected by vacuum filtration and subsequently washed with chilled ethanol to remove any unreacted starting materials or impurities. The isolated compound was then dried to afford the purified Schiff base, and the percentage yield was determined with respect to the calculated theoretical yield [2,6].

4. Spectral Characterisation

Spectral Characterisation The synthesised Schiff base was examined using Fourier transform infrared (FT-IR) and ultraviolet–visible (UV–Vis) spectroscopic methods. FT-IR spectroscopy was used to verify the formation of the azomethine (–C=N–) bond and to identify key functional groups, including the phenolic –OH and methoxy –OCH_3 moieties. UV–Vis spectral analysis was carried out to investigate electronic transitions arising from the conjugated imine framework, and the corresponding absorption maxima (λmax) values were recorded [4,5].

5. In Vitro Antioxidant Activity (DPPH Assay)

The in vitro antioxidant potential of the synthesised Schiff base was assessed using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical scavenging method [8]. A freshly prepared methanolic DPPH solution (0.1 mM) served as the radical source. Stock 4 solutions of the test compound were prepared in methanol and diluted appropriately to obtain concentrations of 20, 40, 60, 80, and 100 µg/mL [9].

Equal volumes of the Schiff base solutions and the DPPH solution were mixed and allowed to react in the dark at ambient temperature for 30 minutes. Following incubation, the reduction in absorbance was recorded at 517 nm using a UV–Visible spectrophotometer. Ascorbic acid was employed as the standard reference compound under the same experimental conditions.

The percentage of DPPH radical scavenging activity was calculated according to the equation given below

$$\% \text{ Inhibition} = \frac{Ao - As}{Ao}$$

where A_0 represents the absorbance of the control and A_s corresponds to the absorbance of the sample.

6. Determination of IC_{50} Value

The IC_{50} value, defined as the concentration of the test compound required to scavenge 50% of DPPH free radicals, was determined from a plot of percentage inhibition against concentration. Linear interpolation was employed to estimate the IC_{50} value, which is reported in µg/mL. This approach allows direct comparison of the antioxidant efficiency of the synthesized Schiff base with previously reported antioxidant systems [9,10].

Results And Discussion

1. Synthesis and Physical Characteristics

Synthesis and Physical Characteristics The condensation of vanillin with the selected aromatic amine under reflux conditions led to the successful formation of a crystalline Schiff base. The reaction proceeded efficiently, yielding the desired product in good isolated yield. The use of ethanol as a solvent and a catalytic amount of glacial acetic acid facilitated efficient azomethine bond formation, consistent with earlier reports on Schiff base syntheses [2,6]. The isolated compound was stable under ambient conditions and exhibited a sharp melting point, indicating reasonable purity and successful completion of the reaction.

The formation of the Schiff base is attributed to nucleophilic attack of the amine nitrogen on the aldehydic carbonyl carbon of vanillin, followed by dehydration to yield the imine linkage. The reaction scheme for the synthesis of the Schiff base is shown in Fig 2. Such reaction pathways are well documented for carbon–nitrogen double bond formation and are characteristic of Schiff base chemistry [1,3].

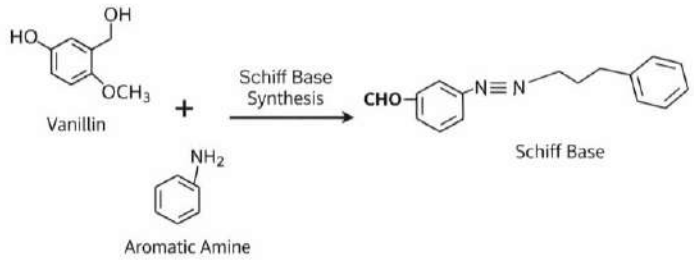


Fig 2 Schematic illustration of the reaction scheme for the synthesis of the Schiff base

2. FT-IR Spectral Analysis

The FT-IR spectrum of the synthesised compound provided clear evidence for Schiff base formation (Fig 3). Aldehydic C=O stretching vibration which is usually visible at around 1680-1700 cm -1 was not present in the spectrum of the synthesised compound. Rather, a new high absorption band was formed at about 1632 cm-1 and this is credited to the azomethine (-C=N-) vibration, a triumphant condensation [4,5].

The presence of an extensive absorption band of about 3402 cm-1 is due to phenolic O-H stretching, which means that the hydroxyl group of the vanillin molecule was not lost. The bands that happened to show up close to 1515 cm-1 were attributed to the C=C stretching vibrations of aromatic compounds, and the one at 1278 cm-1 was linked to the C-O stretching vibrations of the methoxy moiety (Table 1). These assignments are in good agreement with reported FT-IR data for structurally related Schiff base derivatives [6,7].

Table 1. FT-IR Spectral Data

Observed Peak (cm^{-1})	Assignment	Inference
3402	O–H stretching	Phenolic group present
1632	C=N stretching	Azomethine formation
1515	C=C stretching	Aromatic ring
1278	C–O stretching	Methoxy group

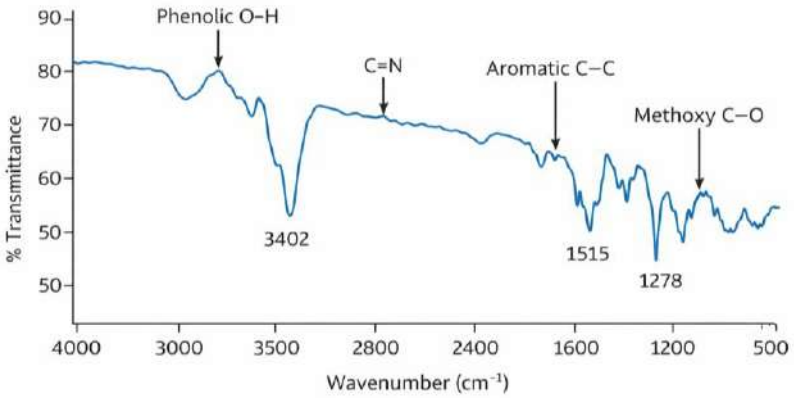


Fig 3 FT-IR spectrum of the synthesised Schiff base

Table 2. Characteristic FT-IR and UV–Visible Absorption Bands of the Synthesized Schiff Base

Technique	Wavenumber / λmax	Assignment	Structural Feature
FT-IR	~1610–1640 cm^{-1}	ν(C=N) stretching	Azomethine linkage
FT-IR	~3400–3500 cm^{-1}	ν(O–H) stretching	Phenolic hydroxyl group
FT-IR	~1500–1600 cm^{-1}	C=C aromatic stretching	Aromatic ring

FT-IR	~1200–1300 cm^{-1}	C–O stretching	Phenolic group
UV–Vis	~280–300 nm	π → π* transition	Aromatic system
UV–Vis	~330–380 nm	n → π* transition	Imine (C=N) chromophore

The observed absorption bands are consistent with the proposed Schiff base structure. The presence of the characteristic azomethine stretching vibration confirms successful condensation between the aldehyde and amine components.

3. UV–Visible Spectral Analysis

The UV–Visible absorption spectrum of the synthesised Schiff base recorded in ethanol had two salient maximum absorption at 278 nm and 342 nm (Fig 4) (Table 2). The lower wavelength absorption is due to the p-p electronic transitions of the aromatic rings and the absorption at 7 at a higher wavelength is due to the n-p transitions involving the lone pair of electrons of azomethine nitrogen [4].

These absorption bands prove the existence of the extended conjugation of the molecule due to the imine bond and the aromatic structure. Other related electronic transitions have been reported on vanillin-derived systems and aromatic Schiff base systems., supporting the structural assignment of the synthesised compound [6,10].

Table 2. UV–Visible Spectral Data

λmax (nm)	Transition
278	π–π* transition
342	n–π* transition

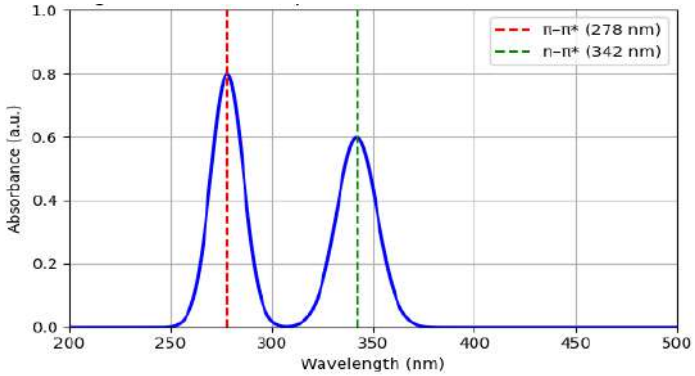


Fig 4 UV-Visible Spectrum of Vanillin-Based Schiff base

4. In Vitro Antioxidant Activity (DPPH Assay)

The antioxidant potential of the synthesised Schiff base was evaluated using the DPPH free radical scavenging assay, and the results are summarised in Table 3 and Figure 3. The synthesised compound demonstrated a concentration-dependent enhancement in DPPH radical scavenging activity. The percentage of inhibition was increasing with concentration, which means that the antioxidant activity is probably related to the existence of the phenolic hydroxyl functional group and conjugated azomethine framework, which could be utilised in the activities of radical quenching by hydrogen atom transfer and resonance stabilisation. The same structureactivity relationship has been reported in phenolic derivatives and Schiff bases systems, and the IC50 value of the synthesised Schiff base was determined as about 50.9 ug/mL, indicating a medium level of antioxidant property in the current study [8,9].

5. IC_{50} Evaluation and Structure–Activity Correlation

IC50 Evaluation and Structure-Activity Correlation IC50 value of the synthesised Schiff base was found to be around 50.9 ug/mL, which represents a moderate antioxidant activity in the present study [8 When it is compared with the already mentioned Schiff base derivatives, which were tested under the same experimental conditions, the value lies within a similar and acceptable range [9,10].

The following antioxidant performance is regulated by structural and electronic properties, such as, molecular conjugation, nature of functional group substitution, and capacity of the compound to donate hydrogen atoms. In particular, Schiff bases derived from phenolic aldehydes such as vanillin have been reported to display improved radical scavenging behaviour, which is consistent with the findings of the present study [6,7,11]. These results further highlight the importance of Schiff base frameworks as useful chemical scaffolds in the development of bioactive molecules with potential relevance to healthcare-related applications [12].

Table 3. IC_{50} Calculation

Concentration (µg/mL)	% Inhibition
20	28.4
40	41.7
60	56.9
80	68.2
100	79.5

IC_{50} Determination

The IC_{50} lies between **40 and 60 µg/mL**.

As per the linear interpolation:

$IC_{50} = 40 + (\frac{50 - 41.7}{56.9 - 41.7}) \times (60 - 40)$

$IC_{50} \approx 50.9$ µg/mL

This result indicates a moderate level of antioxidant activity when compared with commonly used standard antioxidants. The concentration- dependent scavenging behaviour of the compound is illustrated in the DPPH inhibition plot (Fig. 5), confirming its ability to effectively neutralise free radicals as the concentration increases [10].

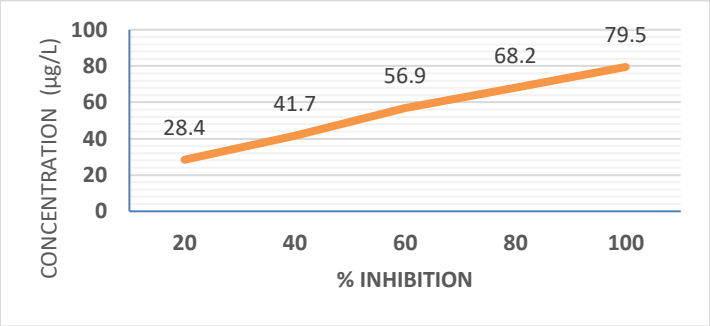


Fig 5 Graph showing DPPH activity

Future Scope

It is possible in the future to synthesize structurally related Schiff bases in order to determine the effect of substituent variation on spectroscopic properties and antioxidant activity. More analytical methods and complementary biological experiments may shed more light on structure-activity relationships. These studies can help create a more detailed study of the reaction of vanillin imine.Bottom of Form

Conclusion

In the study at hand, a condensation reaction was used to produce a vanillin-derived Schiff base in a successful manner. The presence of the structure of the synthesized compound was verified by FT-IR and UV-Visible spectroscopic studies which revealed the presence of the azomethine anion, and the existence of conjugated electronic transitions.

The compound also showed concentration-dependent radical scavenging abilityin the DPPH assay test. The activity that is observed can be ascribed to the presence of the phenolic group and conjugated imine structure in the molecular structure.

Even though the antioxidant activity can be seen to be moderate, the findings suggest that vanillin-based Schiff bases represent convenient organic systems to structure further and assess their functions. Further experiments of greater structural variation and complimentary methods of analysis can help in gaining a more in-depth understanding of the structure-activity relationships.

In general, the findings both indicate the applicability of chemistry of Schiff bases in the study of bioactive organic molecules and offer valuable information on the correlation between 10 molecular structure and antioxidant action [6,9,11]. Though the current study is confined to the in vitro testing, the results reveal that vanillin-derived Schiff bases may be considered as ideal molecular scaffolds to be further structurally adjusted and further biological research in the framework of multidisciplinary healthcare research [12].

Acknowledgements

Acknowledgements The author thanks the laboratory that helped him get facilities to conduct this research.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Data Availability

The data sets created and/or analyzed in the present research such as FT-IR, UV-Vis spectra, DPPH assay data, and IC5O data are accessible to the respective author upon reasonable request. Experimentation procedures and raw information used to justify the results of this research are recorded and can be availed to guarantee reproducibility.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| *Volume-3 Issue-1(I)* | *February-2026* | *ISSN: 3066-0637* | *Website:* https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030126

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19467313

DOI Link:
https://doi.org/10.5281/zenodo.19467313

Volume: 3

Issue: 1(I)

Pp. 120-122

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 14 Jan. 2026

Revised: 24 Jan. 2026

Accepted: 06 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Garipelly, A. (2026). Biofuel Generations and Its Impact on the Environment. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 120–122.
https://doi.org/10.5281/zenodo.19467313

Biofuel Generations and Its Impact on the Environment

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Abstract

Biofuels are renewable energy sources derived from biological materials and are considered viable alternatives to fossil fuels due to their potential to reduce greenhouse gas emissions and enhance energy security. Biofuels are categorized into four generations based on feedstock type and production technology: first-generation (food crops), second-generation (non-food biomass), third-generation (algae), and fourth-generation (genetically engineered organisms with carbon capture). This paper reviews the characteristics of each biofuel generation and critically examines their environmental impacts, including land use, greenhouse gas emissions, biodiversity, water resources, and sustainability. While first-generation biofuels present significant environmental challenges, such as deforestation and food security concerns, advanced generations demonstrate improved sustainability potential. However, technological, economic, and ecological uncertainties remain. The study concludes that future biofuel development must prioritize waste-based feedstocks, efficient production technologies, and integrated environmental management to achieve sustainable energy transitions.

Keywords: *Biofuels, Generations, Renewable Energy, Environmental Impact, Sustainability, Greenhouse Gas Emissions.*

Introduction

The world has been confronted with an energy crisis due to the depletion of finite resources of fossil fuels. The use of fossil fuels as energy is now widely accepted as unsustainable due to depleting resources and also due to the accumulation of greenhouse gases in the environment. Biofuel, any fuel that is derived from biomass – that is, plants, algae, or animal waste. It is considered a source of renewable energy, unlike fossil fuels such as petroleum, coal, and natural gas. CRISIL MI&A Research estimates that India will produce ~147 million tonne (MT) of greenhouse gas (GHG) emissions through conventional fossil fuel-powered passenger vehicles (PVs) in calendar year 2023, marking an increase of 1.4%, amid an unprecedented surge in public transit and shared mobility services led by rapid.

There is a clear need to transition energy dependence from fossil fuels to renewable energy sources to address the unprecedented pace of climate change due to the accumulation of greenhouse gases in the atmosphere. Overwhelming evidence has shown that human activity is the major driver of climate change and that its consequences are impacting food production, migration patterns, economic, and political stability on a global scale. For a sustainable future, alternative energy sources are required to significantly reduce carbon emissions. For this, the Indian government launched the Global Biofuel Alliance (GBA) in 2023. Prime Minister Shri Narendramodi, along with leaders of Singapore, Bangladesh, Italy, USA, Brazil, Argentina, Mauritius and UAE, launched the Global Biofuel Alliance on the sidelines of the G20 Summit in New Delhi on 9, September, 2023. The Global Biofuel Alliance (GBA) is an initiative launched by India as chair of the G20. The alliance hopes to accelerate the Global phase-out of biofuels by facilitating technological progress, intensifying the use of sustainable biofuels, and building robust standards-setting and certification through the participation of a wide range of stakeholders. The cosotium is also acts as a central repository of knowledge and a hub of expertise. The GBA aims to act as a catalytic platform, promoting global collaboration for the development and widespread adoption of biofuels(09 september 2023, 10:30 PM by PIB Delhi). Toyota Kirloskar Motor recently joined hands with the Indian Sugar Mills Association. Six organizations have signed an agreement to promote and create awareness about the use of ethanol as a sustainable biofuel in India. The government of India promotes the use of ethanol as a biofuel on a large scale; by 2025, the Indian Government has set a target of blending twenty percent of ethanol in petrol. By 2025-26, replacing 8.6 crore barrels of petrol with a 20 percent ethanol blend will generate foreign exchange earnings of Rs 30,00 crore for India.

Production of Biofuel:

Today, with environmental policies pushing for a reduction of GHG emissions, aided by recent advances in crop engineering and fermentation processes, bioethanol and biodiesel production have once again become viable and sustainable surrogates for petroleum-based fuels. Bioethanol is derived from corn and sugar cane in the United States and Brazil, respectively, which together account for 84% of the total global production.

India's average ethanol blending rate with petroleum for the calendar year 2023 is estimated at 11.5 percent. The National Biofuels Policy of India, amended in May 2022, strengthens efforts to increase domestic ethanol output from sugarcane and multi-feed stocks by expediting the pace toward blending goals. FAS New Delhi (Post) forecasts India to remain a net ethanol importer for industrial, medical, and beverage usage, and exports to remain limited at 120 million liters due to increased domestic demand and lower sugar feedstock availability. India's biodiesel market remains fragmented and unorganized due to the lack of raw materials, high feedstock prices, and the Indian government's policies, which prioritize ethanol production over other biofuels (USDA-June 20, 2023 Report Number: IN2023-0039). Wood, straw, and domestic refuse are used as a source of heat and energy. Biofuels can also be produced from animal fats, plant wastes, and other organic wastes produced by living organisms.
This process is divided into three categories:

1. **First Generation:** In this generation, biofuels are those that are produced from edible energy crops, sugar-based crops (sugarcane, sugar beet, and sorghum), starch-based crops (corn, wheat, and barley), or oil-based crops (rapeseed, sunflower, and canola). The crops of selected plants are let out freely to absorb the heat from the sun..Later, these crops are refined in factories to produce food products. Once the food products are produced, these crops are refined to produce biofuel. After the production of biofuels, they are collected in tanks and used for a different process.

Environmental Impact:
Advantages:

- Renewable and biodegradable
- Reduction in fossil fuel dependence
- Lower sulfur emissions

Disadvantages:

- Competition with food production
- Deforestation and land use change
- High water requirements
- Soil degradation and fertilizer pollution
- Biodiversity loss

2. **Second Generation:** In this generation, plant dry matter or woody biomass, agricultural residues, and wastes are used to generate biofuel. The Jatropha is a genus of flowering plants in the spurge family. This is a source of biofuel and is widely cultivated in many regions of the world. According to records collected in 2009, Pakistan is the leading country in developing biofuel energy resources globally. Jatropha oil is produced from the seeds of Jatropha curcas, a plant that can grow in wastelands across India, and is considered an excellent source of biodiesel.

Environmental Impact:
Advantages:

- Reduced competition for food supply
- Utilization of waste materials
- Lower greenhouse gas emissions
- Improved sustainability

Limitations:

- High production costs
- Complex processing technologies

3. **Third Generation:** In this Generation Sea algae and microbes are used to generate biofuel. Microalgae are a potential source of renewable energy, and they can be converted into energy such as biofuel, oil, gas, and methane. Since microalgae have high water content, not all biomass energy conversion processes can be applied. By using thermochemical processes, oil and gas can be produced, and by using biochemical processes, ethanol, biodiesel, and bio-hydrogen can be produced.

Environmental Impact:
Advantages:

- High Productivity
- No requirement for fertile land
- Ability to grow in wastewater
- Significant carbon dioxide absorption

Limitations:

- Expensive cultivation and harvesting
- Technological challenges

4. **Fourth Generation Biofuels:** Fourth-generation biofuels involve genetically engineered organisms designed for enhanced fuel production and carbon capture.

Environmental Impact:

Advantages:

- Potential carbon-negative energy
- Integration with carbon capture technologies

Concerns:

- Ethical and ecological risks
- High research and development costs

Comparative Environmental Assessment: Advanced biofuel generations demonstrate progressively improved environmental performance. While first-generation fuels pose significant sustainability issues, later generations reduce land use pressure and greenhouse gas emissions. However, economic feasibility and technological readiness remain key barriers.

Conclusion:

Biofuels are essential for transitioning toward sustainable energy systems. While first-generation biofuels present environmental challenges, advanced biofuels offer promising solutions for reducing emissions and conserving resources. Future research should focus on improving efficiency, reducing costs, and ensuring environmental safety. Policy support and technological innovation are necessary for sustainable biofuel development.

Acknowledgment

I would like to express my sincere gratitude to all those who have contributed to the successful completion of this research work on "Biofuel Generations and Its Impact on the Environment."

I am especially thankful to my institution, Government Degree College, Bhainsa, for providing the necessary academic environment and support to carry out this study.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| *Volume-3 Issue-1(I)* | *February-2026* | *ISSN: 3066-0637* | *Website:* https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030127

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19467377

DOI Link:
https://doi.org/10.5281/zenodo.19467377

Volume: 3

Issue: 1(I)

Pp. 123-126

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 14 Jan. 2026

Revised: 24 Jan. 2026

Accepted: 06 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
P. Latha. (2026). Eat Right for a Better Life: A Survey on Dietary Practices and Lifestyle Patterns. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 123–126.
https://doi.org/10.5281/zenodo.19467377

Eat Right for a Better Life: A Survey on Dietary Practices and Lifestyle Patterns

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Abstract

Nutrition and food chemistry play a crucial interdisciplinary role in promoting human health and preventing life style-related disorders. In this context, a Food Habit Survey was conducted during National Nutrition Week-2025, which adopted the theme "Eat Right for a Better Life." The objective of the survey was to evaluate dietary habits, lifestyle patterns, and nutrition awareness among individuals, emphasizing the chemical and nutritional aspects of food consumption and their impact on health. A structured questionnaire was used to collect responses from 40 participants across different age groups. The survey assessed meal patterns, dietary preferences, intake of fruits and vegetables, consumption of processed and junk foods, water intake, physical activity, and awareness of balanced nutrition. The findings indicate that while a majority of participants follow regular meal patterns and possess basic knowledge of healthy diets, a noticeable reliance on processed and calorie-dense foods persists. Variations in hydration habits and physical activity levels were also observed, reflecting lifestyle diversity. The results highlight the need for integrating nutritional chemistry, food science, and public health education to promote sustainable dietary practices. This study underscores the relevance of interdisciplinary approaches in addressing nutritional challenges and emphasizes the role of nutrition awareness programs in improving food choices and overall well-being. The survey supports the seminar theme by demonstrating how chemistry-based understanding of food and nutrients can contribute to healthier lifestyles and informed dietary decisions.

Keywords: *Food habits, Nutritional Chemistry, Balanced Diet, Lifestyle patterns.*

Introduction

Nutrition is a fundamental determinant of health, growth, and quality of life. The chemical composition of food, nutrient bioavailability, and metabolic processes directly influence immunity, disease prevention, and overall well-being. Rapid urbanization, changing food environments, and sedentary lifestyles have contributed to increased consumption of processed and convenience foods, resulting in nutritional imbalances and lifestyle disorders such as obesity, diabetes, and cardiovascular diseases.

National Nutrition Week–2025 emphasizes the importance of adopting balanced dietary practices through its theme *"Eat Right for a Better Life."* In alignment with this theme, the present study was undertaken to evaluate dietary habits, lifestyle patterns, and nutrition awareness among individuals. The study also highlights the interdisciplinary relevance of chemistry, nutrition, and health sciences in promoting informed food choices.

Review of Literature

Several studies have established a strong link between dietary patterns and the prevalence of non-communicable diseases. Research in nutritional chemistry emphasizes the role of macronutrients, micronutrients, antioxidants, and food additives in maintaining metabolic balance and preventing disease. Excessive intake of refined sugars, trans fats, and processed foods has been associated with oxidative stress and metabolic disorders.

Nutrition education programs have been shown to improve dietary behavior; however, gaps persist due to lifestyle changes, time constraints, and increased availability of fast foods. Recent literature stresses the importance of interdisciplinary approaches combining chemistry, nutrition, and public health to effectively address modern nutritional challenges.

Materials and Methods

1. **Study Design**

A descriptive, questionnaire-based online survey was conducted during National Nutrition Week–2025.

2. **Sample Size**

The study included 40 participants representing different age groups.

3. **Survey Parameters**

The questionnaire assessed:

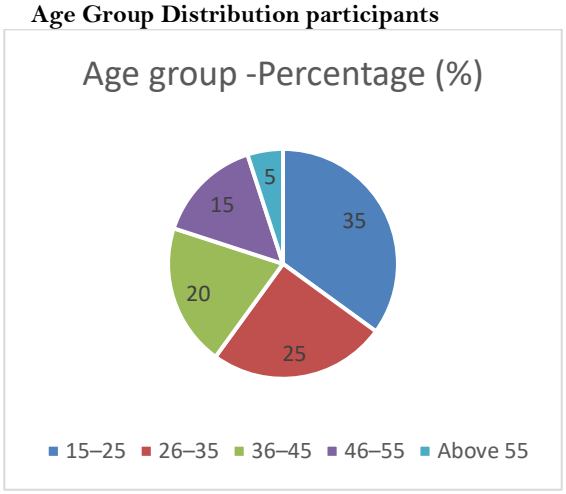
- Age group
- Meal frequency
- Dietary preference
- Fruit and vegetable intake
- Junk/processed food consumption
- Nutrition awareness

4. **Data Analysis**

Responses were analyzed using simple descriptive statistics such as frequency and percentage distribution. Results were presented in tables and charts for clarity.

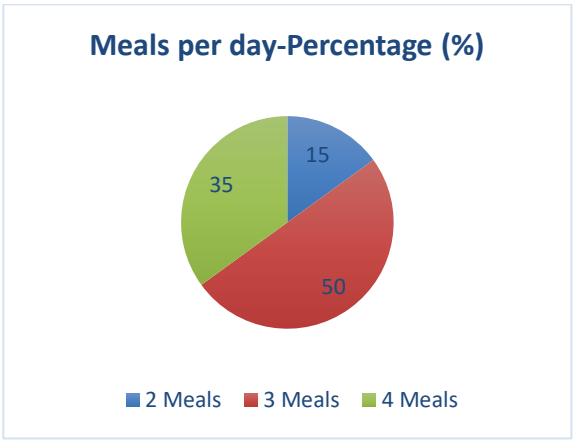
Results

1. **Age Group Distribution participants**



Participants represented diverse age groups, with the highest participation from young adults (15–25 years), indicating greater engagement of younger individuals in nutrition awareness activities.

2. **Meal Frequency**



Half of the respondents consumed three meals per day, indicating relatively regular eating patterns. A significant proportion reported consuming four meals daily, reflecting variations in dietary routines.

3. **Dietary Preferences**

The survey showed a mixed dietary pattern, with 55% non-vegetarians and 45% vegetarians, indicating diverse food choices among participants.

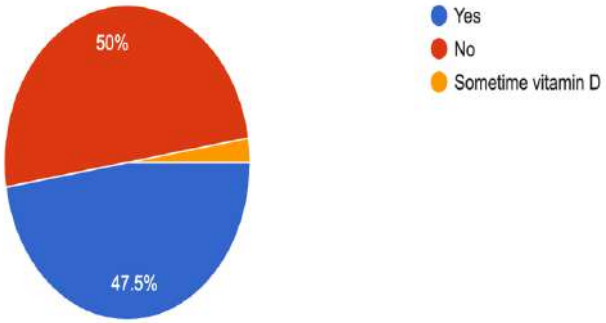
4. **Fruit and Vegetable Intake**

About 60% of participants reported daily consumption of fruits and vegetables, suggesting moderate awareness of balanced nutrition. However, consistency and quantity require improvement.

5. **Junk and Processed Food Consumption**

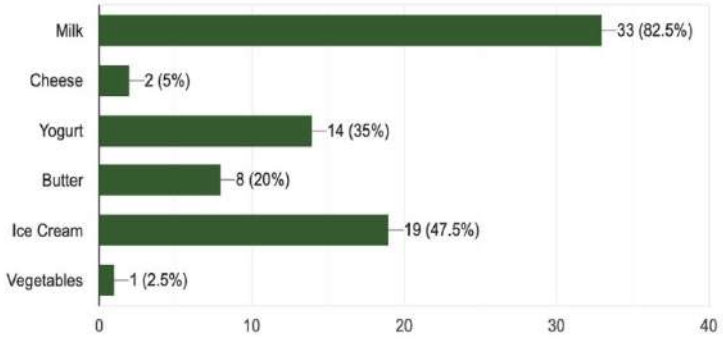
Approximately 30% of respondents frequently consumed junk foods, while 50% consumed them occasionally. This indicates a moderate reliance on processed foods despite awareness of healthy eating.

6. **Vitamins intake on a daily base:**



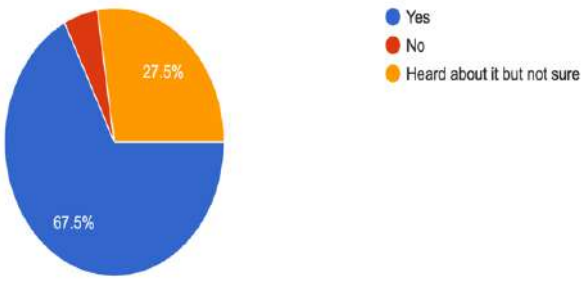
The pie chart illustrates the responses to the question *"Do you take any vitamins on a daily basis?"* among 40 participants. The results show that 50% of respondents do not take vitamins daily**,** indicating that half of the participants rely mainly on regular diet rather than supplements. About 47.5% reported taking vitamins daily**,** reflecting a significant level of awareness regarding micronutrient supplementation. A small proportion of participants reported occasional intake, mainly Vitamin D**,** suggesting selective or need-based supplementation. Overall, the findings indicate moderate awareness of vitamin supplementation, with scope for increased education on the role of essential vitamins in maintaining optimal health.

7. **Consumption of dairy products**



The bar chart shows that **milk is the most commonly consumed dairy product**, reported by **82.5%** of participants, indicating its importance as a primary source of calcium and protein. **Ice cream (47.5%)** and **yogurt (35%)** are also widely consumed, reflecting both nutritional and preference-based choices. **Butter (20%)** is consumed by a smaller proportion, while **cheese (5%)** shows minimal intake. Overall, the results indicate a preference for basic dairy products like milk and yogurt, with limited consumption of high-fat dairy items, suggesting moderate awareness of healthy dietary practices.

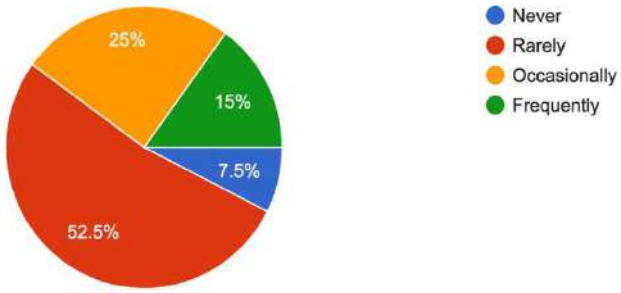
8. **Balanced diet:**



The pie chart indicates that 67.5% of participants are aware of the concept of a balanced diet**,** reflecting good basic nutrition knowledge among the majority. About 27.5% reported that they have heard about a balanced diet but are not fully sure, suggesting partial awareness and the need for clearer understanding. Only a small

percentage responded **"No"**, indicating limited lack of awareness. Overall, the results show a generally positive level of nutrition awareness, while also highlighting the need for focused nutrition education to convert partial knowledge into proper dietary practice.

Fast food consumption



The pie chart illustrates the frequency of fast food consumption among the participants. A majority (**52.5%**) reported consuming fast food **rarely**, indicating a generally cautious approach toward unhealthy food choices. **25%** of respondents consumed fast food **occasionally**, while **15%** reported **frequent consumption**, reflecting a segment at higher risk of poor dietary habits. Only **7.5%** stated that they **never** consume fast food. Overall, the findings suggest moderate fast food intake, with a need for continued awareness programs to reduce frequent consumption and promote healthier alternatives.

Discussion

The findings reveal that although participants demonstrate basic nutrition awareness and follow regular meal patterns, the consumption of junk and processed foods remains prevalent. Regular inclusion of fruits and vegetables reflects positive dietary behavior; however, lifestyle factors such as reduced physical activity and irregular hydration habits pose health concerns.

From a nutritional chemistry perspective, excessive intake of calorie-dense, low-nutrient foods can disrupt metabolic balance and increase the risk of lifestyle disorders. The results are consistent with previous studies emphasizing the need for continuous nutrition education and lifestyle modification strategies

Interdisciplinary Relevance

This study highlights the importance of chemistry in understanding nutrition, including nutrient composition, digestion, metabolism, and the role of food additives. Integrating chemical sciences with nutrition education and public health initiatives can significantly enhance dietary awareness and promote healthier food choices.

Conclusion:

The Food Habit Survey conducted during National Nutrition Week–2025 emphasizes the importance of balanced diets and healthy lifestyles. While awareness of healthy eating exists among participants, its practical implementation remains inconsistent. The study underscores the need for sustained nutrition education programs and interdisciplinary approaches to encourage informed dietary decisions and improve overall well-being.

Acknowledgment

The author expresses sincere gratitude to all the participants who willingly contributed their time and responses to the Food Habit Survey conducted during National Nutrition Week–2025. Their cooperation and valuable inputs made this study possible.

The author is also thankful to the management and staff of Government Degree College for Women, Hussaini Alam, Hyderabad, for providing the necessary support and encouragement to carry out this research work successfully.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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International Journal of Research Studies on Environment, Earth, and Allied Sciences (IJRSEAS)
| Volume-3 Issue-1(I) | February-2026 | ISSN: 3066-0637 | Website: https://eesrd.us

Manuscript ID:
IJRSEAS-2026-030128

OPEN ACCESS

Quick Response Code:

Website: https://eesrd.us

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DOI: 10.5281/zenodo.19481924

DOI Link:
https://doi.org/10.5281/zenodo.19481924

Volume: 3

Issue: 1(I)

Pp. 127-131

Month: February

Year: 2026

E-ISSN: 3066-0637

Submitted: 14 Jan. 2026

Revised: 24 Jan. 2026

Accepted: 06 Feb. 2026

Published: 28 Feb. 2026

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How to cite this article:
Rani, B. S. (2026). Viksit Bharat (Developed India)- An Integrated Perspective of Botany and Chemistry. International Journal of Research Studies on Environment, Earth, and Allied Sciences, 3(1(I)), 127–131.
https://doi.org/10.5281/zenodo.19481924

Viksit Bharat (Developed India)- An Integrated Perspective of Botany and Chemistry

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Abstract

The vision of Viksit Bharat (Developed India) emphasizes sustainable growth, scientific innovation, and environmental responsibility, where Botany and Chemistry play a crucial integrated role. Botany contributes through the improvement of agriculture, conservation of biodiversity, development of high-yielding and stress-resistant crops, afforestation, and the promotion of plant-based solutions for food, medicine, and energy. Chemistry complements these efforts by enabling the development of fertilizers, pesticides, biofertilizers, plant growth regulators, and eco-friendly agrochemicals that enhance plant productivity while minimizing environmental impact. The integration of botanical knowledge with chemical principles supports advancements in green chemistry, phytochemistry, medicinal plant research, biofuels, and biodegradable materials. Together, Botany and Chemistry foster sustainable agriculture, environmental protection, food security, and healthcare innovations, thereby strengthening India's scientific self-reliance (Atmanirbhar Bharat) and contributing significantly to the realization of Viksit Bharat through balanced economic development and ecological sustainability.

Keywords: *Viksit Bharat, Botany, Chemistry, Sustainable Development, Green Chemistry, Agriculture, Biodiversity Conservation, Medicinal Plants, Biofertilizers, Environmental Sustainability*

Introduction

The vision of Viksit Bharat 2047 seeks to transform India into a fully developed nation by the centenary of its independence. This national mission emphasizes economic growth, technological innovation, environmental protection, social equity and Sustainable development. Scientific research plays a fundamental role in this transformation.

Botany focuses on plant science, biodiversity conservation, ecosystem balance and agricultural sustainability. Chemistry provides solutions related to soil fertility, pollution control, renewable energy, environmental protection,. The integration of Botany and Chemistry supports to sustainable agriculture, pollution control, environmental conservation, pharmaceutical development and green technologies, making them essential contributors to national development.

Role of Botany in Sustainable Development

1. **Sustainable Agriculture**

Development of high yielding and stress -resistant crop varieties, Use of plant breeding and biotechnology, Organic farming and sustainable crop management, Promotion of indigenous crop varieties These practices ensure food security and reduce environmental degradation.

2. **Biodiversity Conservation**

Plants maintain ecological balance by producing oxygen, supporting food chains, preventing soil erosion and maintaining water cycles. Conservation of forests and plant species ensures environmental stability.

3. **Carbon Sequestration and Climate Change Mitigation**

Through photosynthesis, plants absorb carbon dioxide and reduce greenhouse gas levels. Afforestation and reforestation programs significantly contribute to climate change mitigation.

4. **Medicinal and Economic Botany**

Research on Medicinal plants, Development of herbal pharmaceuticals, Production of plant based bioactive compounds, Contribution to Ayurveda and traditional medicine systems. This strengthens public health and pharmaceutical innovation.

Role of Chemistry in Sustainable Development

1. **Soil Fertility and Agricultural Chemistry**

Study of soil composition and nutrient cycles, Development of fertilizers and micronutrient supplements, Use of biofertilizers and ecofriendly agrochemicals. These improve crop productivity while reducing environmental impact.

2. **Green Chemistry and Pollution Control**

Green chemistry promotes eco-friendly chemical processes, Reduction of hazardous waste, Development of biodegradable materials, waste recycling technologies. This minimizes environmental pollution

3. **Renewable Energy Development**

Chemistry contributes to biofuel production, hydrogen fuel technology, solar energy materials, Battery and energy storage systems, These reduce dependence on fossil fuels.

4. **Environmental Chemistry**

Water purification technologies, Air pollution monitoring, Waste management solutions, Industrial emission control. These are essential for environmental protection.

Interdisciplinary Integration of Botany and Chemistry

The Integration of these disciplines leads to innovative applications such as Biofertilizer and biopesticide production, Phytoremediation for soil and water pollution, Plant based pharmaceutical development, Biofuel production from plant biomass, Development of biodegradable plastics. These integrated approaches promote sustainability, environmental protection, and economic growth.

However, the concept is scientifically valid and highly relevant. The national vision of Viksit Bharat @ 2047, which aims to transform India into a developed nation by the centenary of its independence, strongly emphasizes sustainability, innovation, and multidisciplinary scientific research. In this context, the integration of botany and chemistry plays a crucial role in achieving environmental sustainability and technological advancement.

Botany contributes significantly to sustainable development through biodiversity conservation, sustainable agriculture, carbon sequestration, and ecosystem stability. Plants serve as primary producers, regulate atmospheric gases, and support ecological balance. Sustainable agricultural practices based on botanical research help ensure food security and environmental protection.

Chemistry, on the other hand, provides essential solutions in soil nutrient management, green chemistry, pollution control, renewable energy, and industrial sustainability. Chemical sciences support the development of eco-friendly fertilizers, biofuels, biodegradable materials, and pollution-reducing technologies.

The integration of botany and chemistry enables innovative approaches such as biofertilizer production, phytoremediation, plant-based pharmaceuticals, and renewable bioenergy development. These interdisciplinary applications contribute directly to environmental protection, agricultural sustainability, and public health.

Therefore, the combined contributions of botany and chemistry are essential for supporting the vision of Viksit Bharat 2047. Their integration strengthens sustainability efforts, promotes scientific innovation, and helps build a developed, environmentally responsible, and self-reliant India.

Importance in Achieving Viksit Bharat 2047

The Viksit Bharat vision emphasizes sustainability, innovation, and scientific development. Botany and chemistry contribute to:

- Food security through improved agriculture
- Environmental protection through pollution control
- Renewable energy development
- Sustainable industrial processes
- Public health through pharmaceutical research

These contributions are essential for building a sustainable and developed nation.

Objectives

The objectives of this study are:

- To examine the contribution of Botany to sustainable development.
- To analyse the role of chemistry in environmental protection and green innovation.
- To evaluate the interdisciplinary integration of Botany and chemistry.
- To assess their importance in achieving the vision of Viksit Bharat @ 2047.

Methodology

This study is based on secondary data collected from scientific journals, academic textbooks, government reports, and environmental sustainability publications, policy documents related to Viksit Bharat. Relevant literature on sustainable agriculture, green chemistry, renewable energy, and interdisciplinary scientific research was reviewed and analysed1

Results and Discussion

1. **Role of Botany in Sustainable Development**

Botanical sciences play an important role in Sustainable Agriculture, Biodiversity Conservation, Carbon Sequestration and Climate Change Mitigation. Plants contribute to oxygen production, carbon dioxide absorption, and ecosystem balance. Scientific advancements in plant breeding and biotechnology help develop improved crop varieties that increase agricultural productivity and food security.

Botanical research also supports biodiversity conservation and ecological sustainability. Forests and plant ecosystems help regulate climate, maintain soil fertility, and protect natural resources.

2. **Contribution of Chemistry to Sustainable Development**

Chemistry plays a significant role in environmental protection and industrial sustainability. Soil chemistry helps improve agricultural productivity through nutrient management and fertilizer development. Green chemistry promotes environmentally friendly chemical processes that reduce pollution and protect ecosystems.

Chemical sciences also contribute to renewable energy development, including biofuels, solar energy, and hydrogen energy. These technologies reduce dependence on fossil fuels and support sustainable energy production.

3. **Interdisciplinary Integration of Botany and Chemistry**

The integration of botany and chemistry provides innovative solutions for environmental sustainability and technological advancement. Important interdisciplinary applications include:

- Development of biofertilizers and biopesticides
- Phytoremediation for pollution control
- Production of plant-based medicines
- Biofuel production from plant biomass
- Sustainable agricultural technologies

These integrated approaches contribute to environmental protection, agricultural sustainability, and public health.

Findings Related to Viksit Bharat@2047

The vision of Viksit Bharat refers to the national mission of transforming India into a fully developed nation by 2047, marking 100 years of independence. This initiative, promoted by the Government of India under the leadership of Narendra Modi, focuses on economic growth, social development, technological advancement, environmental sustainability, and global leadership. The following are the major findings that can be included in a research paper:

i). Economic Growth and Industrial Development

- One of the key findings of the Viksit Bharat initiative is the emphasis on achieving sustained high economic growth. The government aims to transform India into a $30–35 trillion economy by 2047. This involves:
- Strengthening manufacturing through initiatives such as "Make in India"
- Increasing industrial productivity and exports
- Supporting Micro, Small, and Medium Enterprises (MSMEs)
- Promoting innovation-driven economic sectors like artificial intelligence, semiconductors, and renewable energy

As a result, India is witnessing rapid growth in sectors such as electronics manufacturing, automobile production, and digital services. This economic expansion contributes to employment generation and improved national income.

ii). Infrastructure Expansion and Modernization

Infrastructure development is a major pillar of Viksit Bharat. The findings show significant investment in:

- Expansion of Highways and railways
- Railway modernization and high-speed trains
- Airport expansion and regional connectivity
- Smart cities and urban infrastructure
- Digital infrastructure growth

Improved infrastructure enhances connectivity, reduces transportation costs, and promotes regional economic balance. It also attracts foreign direct investment and strengthens national competitiveness.

iii). Digital Transformation and Technological Advancement

India has made remarkable progress in digitalization. The findings highlight:

- Expansion of Digital India initiatives
- Growth of digital payments through UPI
- Increased internet penetration in rural areas
- Use of technology in governance, education, and healthcare

Digital governance improves transparency, efficiency, and accessibility of public services. It also strengthens India's position as a global leader in digital innovation.

iv). Social Development and Human Capital Improvement

Another important finding is the focus on improving the quality of life for citizens. This includes:

- Expansion of education access and skill development programs
- Improvement in healthcare infrastructure and services
- Poverty reduction and financial inclusion through schemes like Jan Dhan Yojana
- Empowerment of women through education and employment opportunities

These efforts contribute to building a skilled and healthy population, which is essential for sustainable development.

v). Environmental Sustainability and Green Growth

Viksit Bharat also emphasizes sustainable development. The findings show strong government commitment to:

- Increasing renewable energy production, especially solar and wind
- Promoting electric vehicles and clean transportation
- Reducing carbon emissions

- Protecting natural resources and biodiversity

India aims to achieve net-zero carbon emissions by 2070, demonstrating its commitment to environmental responsibility.

vi). Governance Reforms and Transparency

Administrative reforms are a key component of Viksit Bharat. The findings indicate:

- Increased use of e-governance systems
- Reduction in corruption through digital monitoring
- Faster delivery of government services
- Greater accountability and transparency in public administration

These reforms improve public trust and enhance institutional efficiency.

vii). Global Leadership and Strategic Position

India's global influence has grown significantly. The findings show:

- Strong participation in global organizations like G20
- Expansion of diplomatic relations and trade partnerships
- Leadership in global issues such as climate change and digital governance

India is emerging as a major global economic and political power.

viii). Challenges and Areas for Improvement

Despite progress, the findings also identify several challenges:

- Income inequality between urban and rural areas
- Unemployment and skill gaps
- Environmental concerns due to rapid industrialization
- Need for stronger education and research systems

Addressing these challenges is essential for achieving the goal of becoming a developed nation.

ix). Measurable Indicators of Progress

Key indicators showing progress toward Viksit Bharat include:

- Rapid GDP growth rate
- Increased digital transactions
- Improved literacy rate
- Reduction in poverty levels
- Expansion of infrastructure networks
- Growth in renewable energy capacity

These indicators demonstrate steady progress toward development goals.

Key Scientific findings:

- Botany ensures food security and biodiversity conservation
- Chemistry supports green technology and pollution control.
- Interdisciplinary research enhances sustainability.
- Integrated scientific approaches accelerate national development

Conclusion

The vision of Viksit Bharat @ 2047 requires strong scientific support from interdisciplinary fields. Botany and chemistry play essential roles in sustainable agriculture, environmental conservation, renewable energy development, pharmaceutical innovation and green industrial processes. Their integration promotes environmental sustainability, economic growth, and scientific self-reliance. Strengthening interdisciplinary research and innovation in these fields is crucial for building a developed, sustainable, globally competitive India by 2047. Therefore, interdisciplinary research combining Botany and chemistry is essential for achieving the goal of a sustainable and developed India.

The findings of Viksit Bharat highlight a comprehensive national strategy focused on economic growth, technological advancement, social welfare, and sustainable development. India's progress in infrastructure, digital transformation, and governance reforms indicates strong potential to achieve developed nation status by 2047. However, addressing inequality, improving human capital, and ensuring environmental sustainability remain critical for the successful realization of this vision.

Acknowledgment

I would like to express my sincere gratitude to all those who have supported and guided me in the completion of this research work on *"Viksit Bharat (Developed India) – An Integrated Perspective of Botany and Chemistry."*

I am especially thankful to my colleagues and academic peers for their valuable suggestions, encouragement, and constructive feedback throughout the preparation of this manuscript. Their insights greatly contributed to improving the quality of this work.

Financial support and sponsorship

Nil.

Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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