FCS

National Seminar

FRONTIERS IN CHEMICAL SCIENCES

November 5-7, 2025

BOOK OF ABSTRACTS

Organized by

DEPARTMENT OF CHEMISTRY
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Message from the

Hon'ble Vice Chancellor

Dear colleagues,

The National Seminar Series, entitled **Frontiers in Chemical Sciences (FCS)**, has been a sincere effort from the teachers and students of the Department of Chemistry over a decade to gather some of the most brilliant researchers from all around the country and to engage them in interdisciplinary discourses for the advancement and dissemination of the most recent developments in Chemical Sciences. It has always brought some of the legendary researchers to the University and has helped the faculty and students of the University imbibe the knowledge, learn methodology and acquire the spirit of open-ended enquiry. This has helped the faculty and the student community to forge meaningful academic relationships, collaborations, and careers in science. During these years, we have witnessed the transformation of several young students venturing into the infinite sea of scientific research, often blossoming into some wonderful careers in chemical sciences.

Continuing this unbroken tradition, the Department of Chemistry is organising **FCS** during November 5-7, with participation of a stellar array of distinguished speakers from all around the country and a strong contingent of students. Let this be a festival of science. I am sure that this edition of FCS too will be impactful, enjoyable and memorable as its earlier versions.

As someone fortunate to be involved in the organisation of all the editions of FCS, I am eagerly looking forward to this year's event. I wish FCS all success. I know that several leading researchers are joining FCS, along with the young researchers and students.

Also, I wish a hearty welcome to all the participants of **FCS** to the University of Calicut.

Prof. P. Raveendran
Vice Chancellor
University of Calicut

Foreword

Every discovery in chemistry begins with a question. It may seem simple or even unexpected, but it has the power to reshape the way we live. From the air we breathe to the technologies we depend on, chemical sciences continue to reveal the fundamental principles that guide both nature and innovation.

At the University of Calicut, the Department of Chemistry has always believed that meaningful progress in science happens through open exchange and collaboration. The seminar series Frontiers in Chemical Sciences (FCS) was initiated with this belief, offering a platform for researchers, educators, and students to come together, share ideas, and explore new directions in chemistry. Over the years, FCS has become a forum that supports academic excellence and strengthens scientific dialogue.

The 2025-26 edition of FCS, to be held from November 5 to 7, continues this tradition. The seminar brings together a wide range of contributions, including 16 invited lectures, 4 keynote lectures, 3 short presentations, 21 oral presentations, and 56 posters. These reflect the energy and diversity that define the field today.

This Book of Abstracts showcases the dedication and curiosity of the contributors. Each abstract is the result of thoughtful research, experimentation, and a shared interest in discovery. The successful preparation of this volume was made possible by the collective efforts of the abstract committee, editorial team, faculty members, scholars, and staff of the Department.

We hope this volume serves not only as a record of the event but also as a reminder that science grows through shared knowledge and a collective pursuit of understanding.

Prof. N. N. Binitha
Head of the Department
Department of Chemistry, University of Calicut

Preface

Chemistry occupies a unique position among the sciences through its ability to bridge and influence diverse disciplines. Advances in Chemical Sciences contribute to society not only through direct applications but also by driving progress in related fields. The increasingly interdisciplinary nature of the subject has given rise to several new areas of research, emphasizing the importance of continuous interaction among scientists. The rapid expansion of these frontiers underscores the importance of regular gatherings where chemists can share ideas and foster collaborations. Established in 1968, the of Chemistry, University of Calicut has made significant contributions to chemical education and research, particularly in northern Kerala. The Department has been fostering such exchanges through its annual national seminar series, *Frontiers in Chemical Sciences (FCS)*. Over the years, FCS has enabled young researchers to interact with leading chemists of the nation, listen to first-hand accounts of scientific breakthroughs, and establish lasting meaningful collaborations that continue to enrich the field.

Continuing this tradition, the Department is organizing *Frontiers in Chemical Sciences (FCS)* during November 5–7. FCS brings together leaders and young researchers to discuss new directions and breakthroughs in Chemical Sciences. The **Book of Abstracts** of FCS features 4 keynote lectures, 16 invited lectures, 3 short invited lectures, 21 oral presentations, and 56 posters. The Department gratefully acknowledges the support of the University authorities, ANRF, KSCSTE, sponsors, and the dedicated efforts of all committee members, faculty, scholars, and staff. We warmly welcome all participants and wish them a fruitful and memorable experience at the University of Calicut during FCS.

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KEYNOTE LECTURES

Electrochemical Interfaces – Studies on Molecular Systems and Materials towards Energy Conversion and Storage

S Sampath[a]

[a]*Department of Inorganic and Physical Chemistry*
Indian Institute of Science, Bangalore

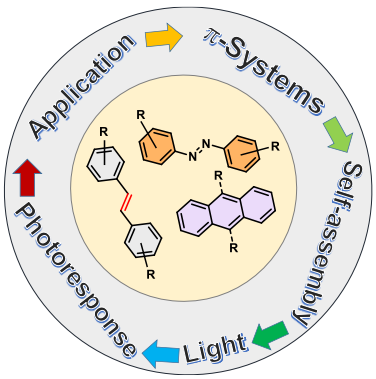
Electrochemical interfaces play a major role in addressing redox reactions of interest to energy conversion and storage. Our group has been interested in understanding various electrochemical interfaces involving solid-solid; solid-liquid and liquid like-liquid interfaces. This includes modified surfaces and new electrode materials comprising molecular systems as well as materials. The present lecture will describe certain attributes of the above, particularly related to systems that are of interest to our group in recent years.

Photoresponsive Supramolecular Assemblies of Small Molecular π-Systems

Ayyappanpillai Ajayaghosh[a]

[a]*SRM Institute of Science and Technology, Kattankulathur, Chennai 603203*
ajayagha@srmist.edu.in

Small molecular π-systems are excellent building blocks for the construction of photoresponsive supramolecular materials, yielding a wide range of structures and functions relevant to smart materials and optoelectronic devices. Integration of photoresponsive units into π-systems are meant to address key challenges in developing responsive and adaptive soft functional materials that dynamically respond to light. Our expertise in supramolecular chemistry and photochemistry helped us in the construction of small molecules based supramolecular assemblies[1,2] for energy transfer,[3,4] chiral inversion,[5] morphology modulation[6] and device application.[7] Recently we have shown that photocycloaddition and photoisomerization reactions can be applied to modulate the Lower Critical Solution Temperature (LCST) of molecular assemblies[8] for the construction of smart windows that can regulate the heat generating near-IR and IR radiations.[9-11] This talk is mainly focused on supramolecular π-systems that exclusively operates on the chemical principles of photoisomerization and photocyclization reactions, and discusses the strategies and directions that govern their design and applications at the nano and microscale.



References

1. Babu, S. S.; Praveen, V. K.; Ajayaghosh, A.; *Chem. Rev*. **2014,** *114*, 1973.
2. Praveen, V. K.; Vedhanarayanan, B.; Mal, A.; Mishra, R. K.; Ajayaghosh, A., *Acc. Chem. Res.* **2020**, *53*, 496.
3. Praveen, V. K.; George, S. J.; Varghese, R.; Vijayakumar, C.; Ajayaghosh, A., *J. Am. Chem. Soc.* **2006**, *128*, 7542.
4. Ajayaghosh, A.; Praveen, V. K.; Vijayakumar, C.; George, S. J.; *Angew. Chem. Int. Ed.* **2007**, *46*, 6260.
5. Gopal, A.; Hifsudheen, M.; Ajayaghosh, *A., Angew. Chem. Int. Ed.* **2012,** *51*, 10505.
6. Mahesh, S.; Gopal, A.; Thirumalai, R.; Ajayaghosh, A., *J. Am. Chem. Soc*. **2012**, *134*, 7227.
7. Das, S.; Okamura, N.; Yagi, S.; Ajayaghosh, A., *J. Am. Chem. Soc*. **2019**, *141*, 5635.
8. Das, S.; Ajayaghosh, A., *Small*, **2025**, e07210
9. Das, S.; Patra, D.; Shankar, S.; Ajayaghosh, A., *Angew. Chem. Int. Ed*. **2022**, *61*, e202207641.

10. Patra, D.; Das, S.; Shankar, S.; Ajayaghosh, A., *Adv. Funct. Mater*. **2024**, 2408014.
11. Patra, D.; Mukhopadyay, R.D.; Ajayaghosh, A., *Angew. Chem. Int. Ed*. **2025**, *66*, e202517868.

Exciton and Biexciton Dynamics in Semiconductor Nanocrystals

K. George Thomas[a]

[a]*School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, Thiruvananthapuram, India*
kgt@iisertvm.ac.in

Developing semiconductor systems for light energy harvesting and optoelectronic applications requires an in-depth understanding of exciton and biexciton dynamics, as well as charge delocalization of photogenerated carriers. Compared to binary (II–VI and III–V) semiconductor nanocrystals (NCs), lead halide perovskite nanocrystals (PNCs) offer several notable advantages due to their defect tolerance. The first part of the presentation will explore the dynamics of bound charge carriers in both binary semiconductor NCs and lead halide PNCs using time-resolved emission spectroscopy.[1] Our findings reveal that trap depth plays a vital role in exciton dynamics in semiconductor quantum dots, whereas the biexciton quantum efficiency in cesium lead bromide PNCs is influenced by the number of facets.[2, 3] In the second part of the talk, I will present strategies to enhance electron delocalization in semiconductor heterostructures and vertex-oriented cube assemblies of perovskites.[4-6] In the last part, I will explain the effect of the plasmonic field on the photoluminescence properties of semiconductor NCs in the presence of Au nanoparticles and Au nanofilms by precisely tuning the distance between the two components.[7-9] I will also discuss how plasmonic fields influence PL lifetimes associated with first and second exciton recombination in a cascade two-photon emission process.

Funding: Nanomission project (DST/NM/TUE/EE-01/2019) of the Department of Science and Technology (DST), Government of India
Acknowledgement: We thank Narayan Pradhan's group for the synthesis of perovskite nanocrystals.

References

1. Vishnu, E. K.; Thomas, E. M.; Prasad, L. ; Thomas, K. G., *J. Phys. Chem. C* **2024**, *128*, 4373-4382.
2. Vishnu, E. K.; Kumar Nair, A. A.; Thomas, K. G., *J. Phys. Chem. C* **2021**, *125*, 25706-25716.
3. Titus, T., *et al.*, *Nano Lett.* **2024**, *24*, 10434-10442.
4. Varghese M. P.; Rajan, A.; Vishnu, E. K.; Titus, T.; Thomas, K. G., *J. Phys. Chem. C* **2024**, *128*, 10945-10954.
5. Garai A., *et al.*, *J. Am. Chem. Soc.* **2023**, *145*, 13989-13999.
6. Thomas, E. M.; Pradhan, N.; Thomas, K. G., *ACS Energy Lett.* **2022**, *7*, 2856-2863.
7. Thomas, E. M.; Cortes, C. L.; Paul, L.; Gray, S. K.; Thomas, K. G., *Phys. Chem. Chem. Phys.* **2022**, *24*, 17250-17262.
8. Paul, L.; Thomas, E. M.; Chemmangat, A.; Gray, S. K.; Thomas, K. G.; *Chem. Sci*. **2024,**

15, 20263-20273.
9. Paul, L. *et al*., *(manuscript under preparation)*

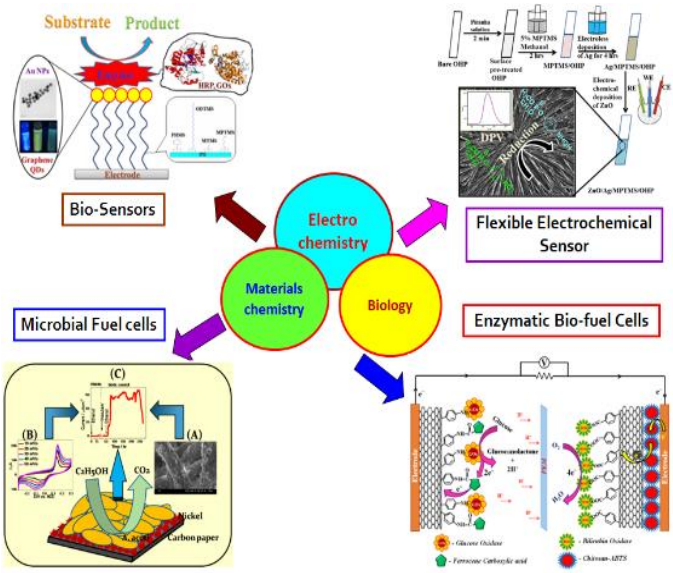
Bioelectrochemistry: A Paradigm Shift from Famous "Frog" Experiment to Flexible (Bio)Sensors to Enzymatic Bio-fuel Cells for Home-based Healthcare Diagnostics

V. Ganesh[a]

[a]*Electrodics and Electrocatalysis (EEC) Division, CSIR – Central Electrochemical Research Institute (CSIR – CECRI), Karaikudi – 630003, Tamil Nadu, India.*
vganesh.cecri@csir.res.in (or) ganelectro@gmail.com

Continued growth of worldwide population in conjunction with highly volatile economics has placed increasing demands for healthcare diagnostics, energy requirements and environmental protection at the forefront globally. Ever increasing climate calamities along with recent pandemic have forced researchers across the globe to find out alternative materials and methodologies for providing solutions to the global issues dominated by healthcare and energy sectors. Modernization of technologies and ever-increasing use of digitization even in the under developed and developing nations like India urge researchers to engineer the materials at molecular level for desired applications, especially in the field of biosensors, energy conversion and storage processes. Huge expenses associated with the modern-day requirements demand researchers to find out alternative, affordable yet beneficial materials and methods to solve some of the issues associated with the above-stated sectors. A successful combination of electrochemistry along with materials chemistry and biology can provide wonderful processes that can be used to solve these crises and provide a way for environmental protection. In general electrochemistry in conjunction with materials chemistry offers a simple, cheap, ease to fabricate devices and provide alternative methodology to engineer the system at either atomic or molecular level to impart desired applications. In this context, this lecture will highlight the significance of multidisciplinary approach primarily using electrochemistry, biology and allied fields. Particularly the experiments performed in our laboratory (***Scheme 1***) in order to tune and enhance the electron transport across the interface using various chemical modification processes will be highlighted. Importantly an example each for electrochemical biosensors, bio-mimics, enzyme catalysis healthcare diagnostics and enzymatic bio-fuel cells [EBFC] applications will be discussed. Moreover, the origin of bioelectrochemistry from the famous "Frog" experiment leading to animal electricity to development of flexible biosensors to smart sensors will be highlighted. Further, some of the recent developments made at our laboratory in the areas of flexible electrodes as bioenergy conversion platforms will also be presented. Interestingly, the energy generated from biochemical reactions and from human excretory fluids utilized for electrochemical biosensing application

will also be discussed. In all these applications, electrochemistry is demonstrated to be a simple yet powerful technique to provide solution to the global issues.



Scheme 1. Pictorial representation of the modification strategies and electrochemical methodologies & materials demonstrated in our laboratory for biosensing and bio-energy conversion applications.

INVITED LECTURES

IL 01

Antimony Lewis Acids

Ajay Venugopal[a]
[a]*Indian Institute of Science Education and Research Thiruvananthapuram*
venugopal@iisertvm.ac.in

Ever since the discovery of the extraordinary acidity of antimony pentafluoride (SbF_5) and its role in the formation of superacids, antimony-based compounds have been recognized for their remarkable electrophilic character.[1] Building on this foundation, our investigations in the past five years explored the design and development of highly reactive antimony species in the +3 oxidation state, with an emphasis on their applications in Lewis acid catalysis.[2-6] This talk outlines key guiding principles that enable the stabilization and tuning of these electrophilic centers through judicious ligand selection and coordination environment control. Structural elucidation using single-crystal X-ray diffraction, complemented by detailed multinuclear NMR spectroscopic analyses, provides strong experimental evidence supporting our proposed hypotheses on electronic structure and reactivity. The catalytic potential of these antimony(III) species is demonstrated through a series of representative transformations, including the deoxygenation of ketones and phosphine oxides, carbonyl–olefin metathesis, and olefin hydroamination. Together, these results establish a versatile platform for advancing main-group element catalysis, highlighting antimony as a promising, tunable, and sustainable alternative to traditional transition-metal-based systems.

References

1. Olah, G. A.; Prakash, S.; Molnar, A.; Sommer, J., Superacid Chemistry (2nd ed.). New York: John Wiley and Sons **2009**.
2. Sharma D.; Benny, A.; Andrews, A. P.; Rajeshkumar, T.; Maron, L.; Venugopal, A., *Nat. Synth.* **2025**, *4*, 462.
3. Benny, A.; Sharma, D.; Ankur; Rajeshkumar, T.; Maron, L.; Venugopal, A., *Chem. Eur. J.* **2023**, 29, e202300588.
4. Sharma, D.; Benny, A.; Sharma, R.; Jemmis, E. D.; Venugopal, A., *Chem. Commun.* **2022**, *58*, 11009
5. Sharma, D.; Balasubramaniam, S.; Kumar, S.; Jemmis, E. D.; Venugopal, A., *Chem. Commun.*, **2021**, *57*, 8889.
6. Kannan, R.; Balasubramaniam, S.; Kumar, S.; Chambenahalli, R.; Andrews, A.P.; Jemmis, E. D.; Venugopal, A., *Chem. Eur. J.*, **2020**, *26*, 12717.

IL 02

Generation of New Heterostructures for Enhanced Electrochemical Water Splitting

Eswaramoorthy Muthusamy[a]

[a]*Chemistry and Physics of Materials Unit (CPMU), School of Advanced Materials (SAMat), Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur P.O., Bengaluru 560064, India.*

Generation of high-purity hydrogen through electrochemical water splitting with zero carbon emissions presents a promising alternative to conventional steam reforming. However, the overall efficiency of this process is limited by the sluggish kinetics of the anodic oxygen evolution reaction (OER). Although noble metal-based electrocatalysts exhibit excellent OER activity, their high cost hinders large-scale deployment. Consequently, various transition metal oxides, sulfides, nitrides, and phosphides have been investigated as cost-effective alternatives; however, issues such as poor conductivity, limited active site accessibility, and inadequate stability across a wide pH range continue to impede their long-term performance. In this talk, I will discuss how the design of new heterostructures, created through simple chemical and electrochemical methods, can substantially enhance catalytic activity and durability for efficient oxygen evolution.

References

1. Zhang, K.; Zou, R., *Small* **2021,** *17*, e2100129.
2. Bhutani, D.; Maity, S.; Chaturvedi, S.; Chalapathi, D.; Waghmare, U. V.; Narayana, C.; Prabhakaran, V. C.; Muthusamy, E., *J. Mater. Chem. A* **2022,** *10*, 22354-22362.
3. Garcés-Pineda, F. A.; Blasco-Ahicart, M.; Nieto-Castro, D.; López, N.; Galán-Mascarós, J. R., *Nat. Energy* **2019,** *4*, 519-525.

IL 03

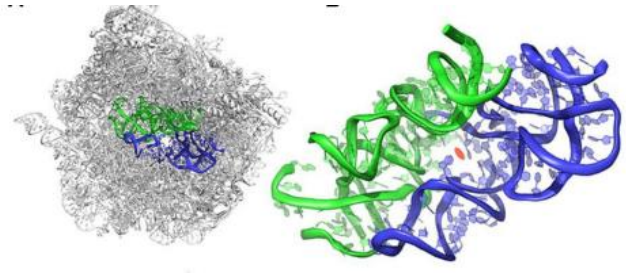
Unravelling the Role of Ribosomes on Life; Concept of Protoribosomes

Franklin John[a]

[a]*Department of Chemistry, Sacred Heart College, Thevara, Kochi-682013*
franklin@shcollege.ac.in

For decades, ribosome was just considered as a passive carrier of genetic information from DNA to the sequence of amino acids in proteins. Recent developments in the field of molecular biology as well as genome sequencing revealed the alternative roles played by RNA. The ribosome consists of two subunits in all species. In bacteria, the subunits are designated as 30S and 50S and together make up the 70S ribosome. Each subunit has three binding sites for the tRNA, termed the A (aminoacyl), which accepts the incoming amino acylated tRNA, P (peptidyl), which holds the tRNA with the nascent peptide chain, and E (exit), which holds the deacylated tRNA before it leaves the ribosome. The 30S subunit has two primary functions in protein synthesis. It discriminates against transfer RNAs that do not match the codon of messenger RNA. Activity of aminoglycoside antibiotics like Neomycin B, is based on specific binding to the 16S rRNA in prokaryotes, thereby inducing miscoding during translation.[1]Combinatorial library synthesis of aminoglycoside mimetics presenting a large structural diversity from a limited number of building blocks will be an attractive approach for finding ligands of new RNA targets arising in the post-genomic era.

Protoribosome is a semi-symmetrical pocket-like region, in 50S subunit of ribosome which accounts for ~6% of the entire large subunit rRNA inprokaryotes. It provides the scaffold for peptide bond formation by anchoring the 3' CCA ends of theribosomal substrates, namely the aminoacyl and the peptidyl tRNA molecules.[2] In order to study theformation of short peptides; esterified derivatives of CCA is being synthesized and tested in biological assays.



References

1. a) Fourmy, D.; Recht, M. I.; Blanchard, S. C.; Puglisi, J. D., *Science*, **1996**, *274*, 1367 371; b) Patel, D. J.; Suri, A. K., *Rev. Mol. Biotechnol*., **2000**, *74*, 39-60; c) Carter, A. P.; Clemons, W. M.; Brodersen, D. E.; Morgan-Warren, R. J.; Wimberly, B. T.; Ramakrishnan, V., *Nature*, **2000**, *407*, 340-348; d) Vicens, Q.; Westhof, E., *ChemBioChem*, **2003**, *4*, 1018-1023
2. Bose, T.; Fridkin, G.; Davidovich, C.; Krupkin, M.; Dinger, N.; Falkovich, A. H.; Peleg, Y.; Agmon, I.; Bashan, A. and Yonath, A., *Nucleic acids research*, **2022**, *50*, 1815-1828.

IL 04

Greening Organic Reactions *via* Polymer Immobilized Catalysts

Anas Saithalavi[a]

[a]*School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala-686560*
anas@mgu.ac.in

With the rapid development of "green" chemistry, researchers are highly focused on selecting more sustainable and eco-friendly synthetic routes and materials. Therefore, efforts leading to the development of novel recyclable catalytic systems offering higher reusability and sustainability are very much demanding. Among those, the heterogenization of homogeneous catalysts onto suitable support materials such as polymers has received larger attention due to several advantages. In recent years, polyacrylonitrile (PAN) has been identified as an ideal choice as it offers immense post-functionalization potential due to the presence of reactive nitrile (CN) functionality.[1] Our work mainly focuses the development of novel heterogeneous polymer supported transition metal (Pd, Cu, Fe, Ni etc) catalysts *via* immobilization of the metal salts over synthetically modified polyacrylonitrile (mPAN)and exploring their applications in promoting various organic reactions.[2-9] Notably, these catalysts demonstrated excellent recyclability and reusability, by maintaining substantial stability and activity over several successive runs.

References

1. Sruthi, P. R.; Anas, S., *J. Poly. Sci.*, **2020**, *58*, 1039.
2. Sruthi, P. R.; Sarika, V.; Arya, S.; Krishnan, A.; Anas, S., *Inorg. Chim. Acta*., **2020**, *502***,** 119305.
3. Saranya, T. V.; Sruthi, P. R.; Veena, R.; Anas, S., *J. Organomet. Chem.*, **2021,** *937*, 121733
4. Sruthi, P. R.; Nimmi, P. P.; Babu, S. S.; Anas, S., *ChemistrySelect*, **2022**, *7*, e202104273.
5. Sruthi, P. R.; Roopak, R.; Anas, S., *ChemistrySelect*, **2023**, *8*, e202204374.
6. Rubina, S.; Vineetha, P. K.; Anas, S., *J. Photochem. Photobiol. A: Chem*., **2024**, *449*, 115410.
7. Arya, S.; Asiya, A. S.; Anas, S., *New J. Chem.*, **2024**, *48*, 17385.
8. Sruthi, P. R.; Malini, S.; Silpa, S.; Anas, S., *J. Organomet. Chem*., **2025**, *1025*, 123452.
9. Rubina, S.; Arya, S.; Anas, S., *ChemistrySelect*, **2025**, *10*, e03274.

IL 5

Orthogonal Donor–Acceptor Architectures in Macromolecule, Nanographene and Graphene Nanoribbon

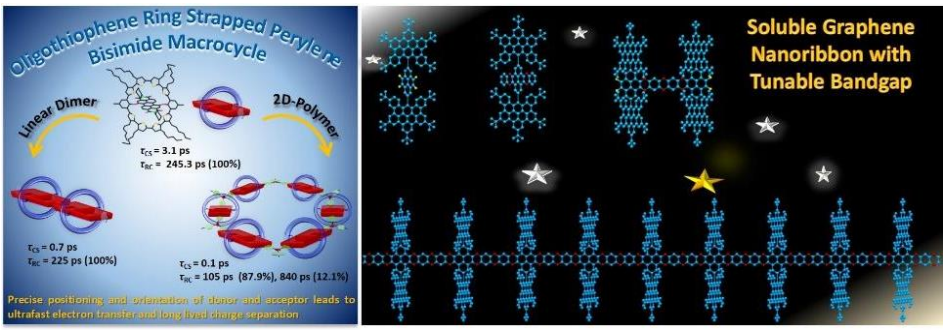
Santhosh Babu Sukumaran[a,b]

[a]*Organic Chemistry Division, National Chemical Laboratory (CSIR-NCL), Dr. Homi Bhabha Road, Pune-411008*

[b]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201 002, India*

sb.sukumaran.ncl@csir.res.in

Orthogonal donor–acceptor (D–A) architectures offer a flexible design approach in π-conjugated chemistry, positioning electron-donating and accepting units at perpendicular angles to influence electronic coupling and excited-state dynamics.[1] Unlike traditional coplanar D–A systems that enhance π–π overlap, orthogonal configurations limit conjugation along one axis while allowing cross-conjugated interaction between molecular orbitals. This spatial decoupling results in distinct photophysical and electronic properties, such as prolonged charge-transfer states and reduced recombination. In this context, donor-acceptor-linked π-conjugated macrocycles are inspiring modular building blocks that allow both light harvesting and excitation energy transfer and electron transfer. Our recent findings in the area of donor-strapped PBI-based macrocycles revealed the importance of new molecular designs in extending the charge-separated state and opportunities for further functionalization of macrocycles.[2] The concept of orthogonality has been extended to nanographene and graphene nanoribbons to impart donor-acceptor features that tune the band gap, and thereby influence photophysical and redox properties.[3]



References

1. Giribabu, L.; Ashok Kumar, A.; Neeraja, V.; Maiya, B. G., *Angew. Chem. Int. Ed.* **2001**, *40*, 3621-3624.
2. Freeman, D. M. E.; Musser, A. J.; Frost, J. M.; Stern, H. L.; Forster, A. K.; Fallon, K. J.; Rapidis, A. G.; Cacialli, F.; McCulloch, I.; Clarke, T. M.; Friend, R. H.; Bronstein, H., *J. Am. Chem. Soc*. **2017**, 139, 11073–11080.

3. Veer, S. D. ; Wakchaure, V. C.; Asokan, K.; Dixit, R.; Goswami, T.; Saha, R.; Gonnade, R.; Ghosh, H. N.; Babu, S. S., *Angew. Chem. Int. Ed.* **2023**, *62*, e202212934.
4. Veer, S. D.; Goswami, T.; Ravindranathan, S. H.; Gonnade, R.; Kharbanda, N.; Ghosh, H. N.; Babu, S. S. *Org. Chem. Front.* **2023**, *10*, 5099–5107.
5. Unpublished results.

IL 06

Sustainable Transformation of Biomass Components to Platform Chemicals using Heterogenous Composite Catalysts

A. Sakthivel[a*], M. Bhavisha, N. P. Nimisha, K. K. Shabana, P. Aswin, S. N. Soumya

[a]*Inorganic Materials and Heterogeneous Catalysis Laboratory, Department of Chemistry, Central University of Kerala, Kasaragod, Kerala 671325, India.*
[*]*sakthivelcuk@cukerala.ac.in*/sakthiveldu@gmail.com

Keywords: Biomass, Heterogeneous catalysts, Perovskite oxide, Hydrotalcite, Zeolite, Aluminophosphate

The rapid exhaustion of non-renewable energy resources has intensified the need for advanced catalytic technologies to harness renewable alternatives, particularly biomass. Analogous to the petrochemical industry, these biomass-based materials can serve as feedstocks for producing various platform molecules for fine chemicals and fuels. Efficient valorization of biomass-derived platform molecules requires a robust catalytic system endowed with multifunctionality, high stability, and tunable reactivity, which is the focus of current research efforts. In this regard, our research team focuses on developing sustainable multifunctional catalysts derived from mixed metal oxides, bimetallic hydrotalcite (HT) catalysts, metal–metal oxide-encapsulated zeolites, and zeolite–metal–oxycarbide composites. The developed catalyst systems were systematically characterized by spectroscopic and analytical methods. The resultant materials were investigated for the conversion of various biomass components (furfural, eugenol, cinnamyl alcohol, levulinic acid, etc.) into platform molecules for fuel additives and fine chemicals.

For example, the exsolved Ni–Ru alloy on the surface of the $SrFe_{0.9}Ni_{0.05}Ru_{0.05}O_{3-\delta}$ (SFNR1R) perovskite catalyst was found to be effective for the hydrogenation of furfural. The uniform distribution of Ni–Ru species on the oxygen-deficient perovskite-derived brownmillerite catalyst facilitated complete conversion of furfural (99%) with selective formation of furfuryl alcohol (91%).[1] Similarly, Si- and Ru-co-doped $SrFeO_{3-\delta}$ was demonstrated as an efficient catalyst for chemoselective hydrogenation of furfural (95%) to furfuryl alcohol. The synergistic effect of nickel and oxygen vacancies in Ni-doped $LaAlO_3$ facilitated hydrogenation of cinnamaldehyde to hydrocinnamyl alcohol (CAL conversion of 98% with 96.5% HCOL selectivity).[2] On the other hand, highly dispersed metallic ruthenium on an HT support exhibited promising activity in 5-hydroxymethylfurfural oxidation in an aqueous medium (98.3% conversion), leading to the formation of 2,5-furandicarboxylic acid.[3] Furthermore, the framework composite material molybdenum-oxycarbide-stabilized SAPO-37

zeolite was found to be a promising catalyst for MTBE synthesis (83%).[4] Likewise, the zirconia–SAPO- 37 composite was identified as a potential catalyst for the production of ethyl levulinate (EL) from furfuryl alcohol with a 99% yield.[4]

In summary, these multifunctional heterogeneous catalysts demonstrate great promise for the sustainable conversion of biomass into value-added chemicals.

The authors thank DST-SERB-CRG/2023/001107,for the financial assistance.

References

1. Bhavisha, M.; Sakthivel, A., et al., *Sustain. Energy Fules*, **2024**, *8*, 2839-2849.
2. Bhavisha, M.; Sakthivel, A., et al., *ChemCatChem.*, **2025**, *17*.
3. Aswin, P.; Sakthivel, A., *Chem. Asian J.*, **2025,** *20*.
4. Shabana, K. K.; Sakthivel, A., et al., *Chem. Commun.*, **2024,** *60***,** 8688; 2025, 61, 1136.

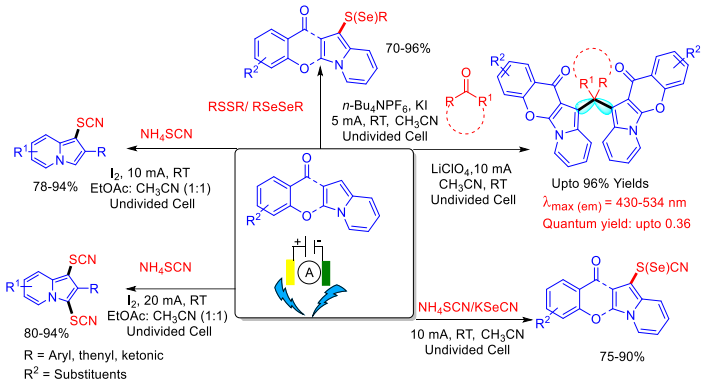
IL O7

Site-Selective Electrochemical Functionalization of Indolizine Frameworks Enabled by N-Centered Radical Translocation

Satpal Singh Badsara[a]

[a]*MFOS Laboratory, Department of Chemistry, Institute of Science, Banaras Hindu University (BHU), Varanasi, Uttar Pradesh, India.*
satpals.badsara4@bhu.ac.in

Electro-organic synthesis provides a sustainable approach that utilizes electrons as reagents for molecular transformations, thereby eliminating the need for excess reagents.[1] Our research group has recently developed various electrochemical approaches for the functionalization of indolizine moieties *via N*-centered radical translocation. During my presentation, I will provide a detailed discussion of these approaches.[2]



References

1. (a) Wang, Y.; Dana, S.; Long, H.; Xu, Y.; Li, Y; Kaplaneris, N.; Ackermann, L. *Chem. Rev.* **2023**, *123*, 11269-11335. (b) Kingston, C.; Palkowitz, M. D.; Takahira, Y.; Vantourout, J. C.; Peters, B. K.; Kawamata, Y.; Baran, P. S. *Acc. Chem. Res.* **2020**, *53*, 72-83. (c) Badsara, S. S.; Ucheniya, K.; Chouhan, A.; Gurjar, A. Chem. Rec. 2025, 00, e202500092. (d) Jat, B; Yadav, D. K.; Badsara, S. S.; Sharma, S. *Org. Biomol. Chem.* **2025**, *23*, 4846-4854.
2. (a) Jat, P. K.; Badsara, S. S. *J. Org. Chem.* **2024**, *89*, 12263-12276. (b) Ucheniya, K.; Jat, P. K.; Chouhan, A.; Yadav, L.; Badsara, S. S. *Org. Biomol. Chem.*, **2024**, *22*, 3220-3224. (c) Jat, P. K.; Yadav, L.; Chouhan, A.; Ucheniya, K.; S. S. Badsara, *Chem. Commun.*, **2023**, *59*, 5415-5418. (d) Chouhan, A.; Ucheniya, K.; Yadav, L.; Jat, P. K.; Gurjar, A.; Badsara, S. S. *Org. Biomol. Chem.*, **2023**, *21*, 7643-7653. (e) Jat, P. K.; Dabaria, K.; Bai, R.; Yadav, L.; Badsara, S. S. *J. Org. Chem.*, **2022**, *87*, 12975-12985.

IL 08

Low Dimensional Materials Supported Single Atom Catalysts for Ambient Temperature CO Oxidation

Elambalassery G. Jayasree[a]

[a]*Dept. of Applied Chemistry, CUSAT, Kochi-22*

jelambal@cusat.ac.in

The idea that isolated single atoms on a support selectively drive a reaction has led to the much fascinating research field of single atom catalysis. Nowadays, single atom catalysts (SAC) have successfully been employed in various applications including organic synthesis, air or water pollutant removal or the manufacturing of novel energy resources. Designing suitable and selective SAC towards the activation of small molecules including environmental pollutants such as CO, CO_2, and NO_x is of utmost importance. We have investigated SAC supported on various low dimensional materials such as main group nanorings and MXenes towards CO oxidation at ambient conditions (Figure shown below). DFT studies are employed to unravel the electronic structure and stability of SAC, SAC mediated reaction mechanism and corresponding energy barriers. The results of our study will be detailed in the presentation.

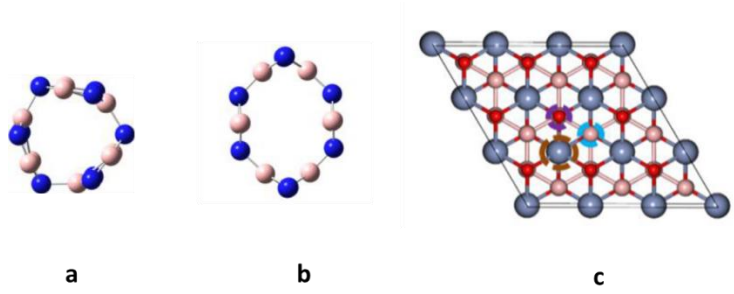


Figure 1. a, b: Nanorings of various sizes, c: Cr based Mxene

IL 09

Wettability Control in Electrochemical Systems: Why it Matters and How to Leverage it

Pradeep Kumar Sow[a]

[a]*Department of Chemical Engineering, BITS Pilani, K.K. Birla Goa Campus*

Surface wettability plays a pivotal role in electrochemical systems because both are fundamentally governed by processes occurring at the solid–liquid interface. Wettability determines the extent and nature of this interface, influencing liquid affinity, interfacial contact, and consequently, the effective area available for charge transfer. Enhanced wettability can increase the active interfacial area, thereby impacting electrochemical reaction kinetics, mass transport, and overall system performance. Recognizing this interdependence between electrochemistry and surface science opens opportunities for designing improved interfaces, materials, and device architectures. This talk will present a concise overview of how surface wettability affects electrochemical behaviour, techniques to evaluate and quantify wettability, and strategies for tuning surface properties. Selected case studies will highlight how engineered wettability has been harnessed to enhance electrochemical processes and develop novel applications.

IL 10

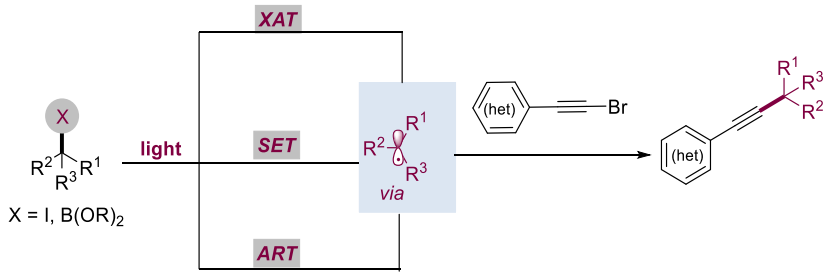
Synthesis of Internal Alkynes *via* SET, XAT and ART

Veera Reddy Yatham[a]

[a]*School of Chemistry, Indian Institute of Science Education and Research, Thiruvananthapuram 695551, India.*

Keywords: Light, Alkyl halides, Boronic acids, Alkynes

Alkynes are important and versatile building blocks in organic chemistry frequently appearing in natural products, bioactive compounds. The internal alkyne moiety allows numerous modifications for the synthesis of pharmacophores, fine chemicals and agrochemicals. Therefore, the construction of internal alkynes using a variety of alkyl radical precursors such as has alkyl carboxylic acids and its derivatives, 4-alkyl-substituted Hantzsch esters (HEs), alkyl NHP esters, alkyl Katritzky salts, alkyl thianthrenium salts, alkyl iodides, alkyl-BF_3k, alkyl-Bpin and using excess of hydrocarbons have been reported using acetylenic sulfone or ethynylbenziodoxolone (EBX) as an alkynylating reagent. However, most of the developed methods produce large amounts of by-products that are generated either from alkyl radical precursor or alkynylating agent. Also, halo alkynes are important and widely used intermediates in synthetic chemistry. It has also been shown that these haloalkynes serve as effective alkynylating agents, thanks to their atom economy and ease of availability. In the present lecture I will discuss photoinduced synthesis of Internal alkynes via the concept of Halogen atom transfer (XAT), Single electron transfer (SET) and Amino radical transfer (ART).[2]



Scheme 1. Photoinduced synthesis of internal alkynes

References

1. Vaillant, F. L.; Waser, J. *Chem. Sci.*, **2019**, *10*, 8909–8923.
2. Ge, D.; Wang, X.; Chu, X. –Q., *Org. Chem. Front.* **2021**, *8*, 5145–5164.
3. Bisoyi, A.; Tripathy, A. R.; Poolamanna, R.; Yatham, V. R., *Org. Lett.* **2025**, *27*, 9042–9048.
4. Tripathy, A. R.; Rahmathulla, A. R.; Kumar, A.; Jha, A. K.; Yatham,V. R., *Org. Lett.* **2022**, *24*, 5186–5191.
5. Bisoyi, A.; Behera, A.; Yatham, V. R., *unpublished results.*

IL 11

Chiral Light Emitting Molecules and Nanomaterials

Jatish Kumar[a]

[a]*Department of Chemistry, Indian Institute of Science Education and Research (IISER) Tirupati, Tirupati 517619, Andhra Pradesh, India*
jatish@iisertirupati.ac.in

Chirality is ubiquitous in nature and chiral molecules have fascinated researchers over decades due to the vast applications offered by these systems. Recent advances in nanoscale chirality have rejuvenated the field and has captivated research interest. Chiral nanomaterials are synthesized through: (i) the synthesis of intrinsically chiral nanoparticles, (ii) chiral induction using chiral ligands, and (iii) template assisted methods. Chirality is investigated using circular dichroism (CD) spectroscopy which investigates the ground state chiral properties. Of late, research interest has focused attention on chiral light emitting molecules and materials due to their vast application in field of display devices, data encryption, chiral biosensing and bioimaging. A reactively new technique that investigates the excited state optical activity is circularly polarized luminescence (CPL). Our recent attempts on the synthesis of chiral emissive nanomaterials, and the investigations on their excited state optical activity CPL will be discussed. CPL has gained tremendous attention due to its relevance to both fundamental and applied research. Working in this direction, we have recently demonstrated CPL in organic molecules as well as different class of nanomaterials. Intrinsic, ligand induced, and templated chirality in molecules as well as in nanomaterials will form the topic of discussion. Our recent attempts towards understanding the fundamentals of optical activity in molecules and nanomaterials and their potential applications in various fields will be discussed in brief.

References

1. Dutta, C.; Mandal, A.; Shukla, A.; Hemaprabha, E.; Nakashima, T.; Kumar, J., *Angew. Chem. Int. Ed.*, **2025**, *64*, e202411554.
2. Dutta, C.; Kumar, J., *Chem. Sci.*, **2025**, *16*, 18713–18721.
3. Dutta, C.; Natarajan, R. V.; Kumar, J., *Chem. Sci.*, **2025**, *16*, 1722–1729.
4. Jadhav, A.; Cheran, A.; Dutta, C.; Kumar, P.; Pujala, R. K.; and Kumar, J., *ACS Mater. Lett.*, **2025**, *7* 508.
5. Jadhav, A. B.; Cheran, A.; Dutta, C.; Marydasan, B.; Kumar, J., *J. Phys. Chem. Lett.*, **2024**, *15*, 8125.
6. Nalavadath, S. T.; Maniappan, S.; and Kumar, J., Nanoscale, **2024**, *16*, 13571.
7. Maniappan, S.; Dutta, C.; Solís, D. M.; Taboada, J. M.; and Kumar, J., *Angew. Chem. Int. Ed.*, **2023**, *62*, e202300461.

IL 12

Self-Sensing Polymeric Electrochemical Motors: Towards Biomimetic Artificial Muscles and Proprioceptive Devices

Yahya A. Ismail[a,*]

[a]*Centre for Advanced Materials, Dept of Chemistry, University of Calicut*
aiyahya@uoc.ac.in

Understanding the fundamental mechanisms behind brain functions, proprioception, and self-sensing muscular actuation remains one of the most compelling challenges in science. Conventional models, based on systems of constant composition, fail to capture the dynamic, reactive nature of biological systems. To bridge this gap, we propose conducting polymers as reactive model materials capable of mimicking the coupled sensing–actuation behavior of biological muscles. These materials, driven by low electrical potentials, undergo reversible compositional and conformational changes during electrochemical reactions—behaviors strikingly similar to those of natural muscles. Conducting polymers act as macromolecular electrochemical motors in which the polymer chains, ions, and solvent cooperatively participate in charge-driven reactions. The electrical energy consumed during these processes inherently encodes information about the surrounding chemical, electrical, and thermal conditions, enabling in situ self-sensing without the need for additional sensors or wiring. The same two electrical connections simultaneously transmit actuation (current and charge) and sensing (potential and energy) signals, analogous to the communication between the brain, motor neurons, muscles, and sensory neurons. This unified sensing–actuation mechanism offers quantitative insight into biological phenomena such as muscle fatigue and neural feedback.

Our studies demonstrate that the self-sensing property is a general characteristic of all conducting polymers and can be exploited for developing soft, multifunctional, and adaptive devices. These can include biomimetic artificial muscles, self-sensing electrochemical energy storage systems, soft actuators, smart membranes etc. Various materials and technologies employed will be discussed. The exploration of conducting polymers as biomimetic, reactive materials opens a new paradigm in designing polymeric motors and multifunctional electrochemical systems capable of sensing, actuation, and adaptation—key steps toward realizing artificial organs and next-generation smart technologies.

IL 13

New Advances in Atomically Precise Silver and Copper Nanoclusters

Sukhendu Mandal[a]

[a]*School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, Thiruvananthapuram, Kerala, India-695551*
sukhendu@iisertvm.ac.in

Atomically precise metal nanoclusters (NCs), a new class of materials are composed of tens to hundreds of metal atoms in the core and possess unique structures, high stability, and attractive properties. Built on the significant success of Au NCs, Ag and Cu NCs have recently received increasing attention. Synthesis and structural elucidation of these NCs are challenging because the zero-valent oxidation states of Ag and Cu are very reactive and prone to oxidization.[1] We have designed a new strategy to synthesize Ag and Cu NCs and then correlated their structure-property relationship. Here, we will discuss the following: (a) A new Ag-S NC $[Ag_{50}S_{13}(S^tBu)_{20}][CF_3COO]_4$ with its unique hcp Ag_{14} kernel and Ag_{36} Keplerian shell-based structural architecture and its photoresponsivity;[2] (b) Ag_{12}-based two-dimensional cluster-assembled materials and their optoelectronic properties;[3](c) Presence of unique structural geometry in Cu_{18} and Cu_{29}-based NCs (Figure 1).[4]

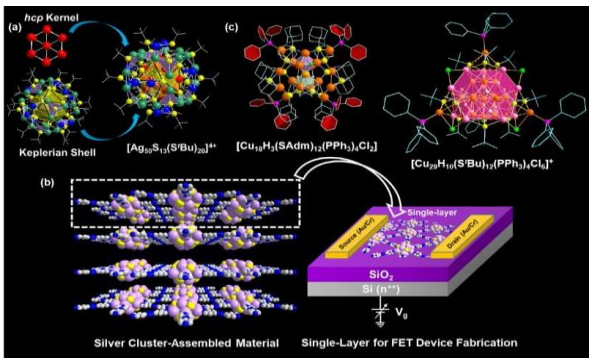


Figure1: Structural illustration of the newly synthesized atom-precise Ag and Cu NCs.

References

1. Yang, J.; Jin, R., *ACS Mater. Lett.*, **2019**, *1*, 482-489.
2. Biswas, S.; Das, A. K.; Reber, A. C.; Biswas, S.; Bhandary, S.; Kamble, V. B.; Khanna, S. N.; Mandal, S., *Nano Lett.*, **2022**, *22*, 3721-3727.
3. Das, A. K.; Biswas, S.; Kayal, A.; Reber, A. C.; Bhandary, S.; Chopra, D.; Mitra, J.; Khanna, S. N.; Mandal, S., *Nano Lett.*, **2023**, *23*, 8923-8931.
4. Das, A. K.; Biswas, S.; Wani, V. S.; Nair, A. S.; Pathak, B.; Mandal, S., *Chem. Sci.*, **2022,** *13*, 7616-7625.

IL 14

In Situ Engineering of Conducting Polymer Nanomaterial Hybrids at Liquid/Liquid Interfaces

Mini Mol Menamparambath[a]

[a]*National Institute of Technology Calicut*
minimol@nit.ac.in

Conducting polymers are increasingly hybridized with other materials to address their inherent functional limitations when compared to metallic or inorganic counterparts. Among the various synthesis approaches, liquid/liquid (L/L) interface-assisted methods have emerged as a simple yet powerful strategy for designing fully tunable metamaterials suited for diverse applications. The spontaneous adsorption of nanostructures at quasi-two-dimensional interfaces is energetically favourable, driven by the reduction in interfacial tension, surface area, and overall Helmholtz free energy. A simple in situ liquid/liquid polymerization method is presented for the first-time synthesis of silver-doped hollandite manganese oxide (Ag-HMO) supported on polypyrrole (PPy). This novel approach enables the formation of α-MnO_2 attached to PPy oligomers under mild temperature conditions. Silver ions (Ag^+) are then intercalated in situ into the 2 × 2 tunnel structure of α-MnO_2, resulting in the formation of Ag-HMO incorporated within the PPy matrix. The fundamental principles behind nanostructure adsorption and the formation of hierarchical architectures at interfaces, with an emphasis on practical insights will be discussed during the conference.

References

1. Kaladi Chondath, S.; Bansal, L.; Veluthath Rethnakumaran, A.; Davison, D.; Puthiyaparambath, M. F.; Chatanathodi, R.; Kumar, R.; Menamparambath, M. M. *Small Methods* **2025**, *9*, 2401699.
2. Menamparambath, M. M.; et al. *ACS Mater. Au* **2024**, *4*, 115–128.

IL 15

Catalytic Oxidation of Ethylene: In Pursuit of Room Temperature Activity

Dinesh Jagatheesan[a]
[a]*Department of Chemistry*
IIT Palakkad

Agricultural produce, such as Fruits and vegetables, stored in a warehouse, are prone to decay rapidly in the presence of ethylene. Transition metal oxide (TMO) catalysed catalytic oxidation of ethylene to CO_2 is an essential and scalable strategy to increase the storage time. There are multiple methods to enhance the concentration of oxygen vacancies (O_V) in TMOs, which are one of the active sites in TMO-catalysed ethylene oxidation. In this talk, I will discuss various efforts we have made in recent years to improve the catalytic activity of TMO at ambient conditions.

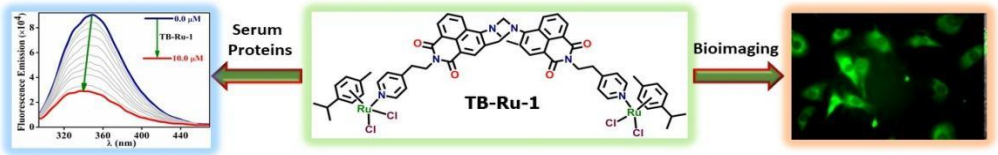
IL 16

From Molecular Design to Function: Supramolecular Fluorescent Systems of Amino- 1,8-Naphthalimide-Tröger's Base Scaffolds

Shanmugaraju Sankarasekaran[a]

[a]*Department of Chemistry, Indian Institute of Technology Palakkad, Kerala, India.*
shanmugam@iitpkd.ac.in

Self-assembly refers to the spontaneous organization of components into well- defined groups based on the information inherent in the components themselves.[1] In recent years, we have focused on the rational design and synthesis of amino-1,8-naphthalimide- derived Tröger's bases (TBNaps) as fluorophores, using them as bifunctional supramolecular scaffolds to create hierarchical structures and new materials for applications in material and medicinal chemistry.[2] TBNaps are intriguing chiral frameworks, consisting of a methano-1,5- diazocine ring fused with two orthogonally positioned 1,8-naphthalimide molecules, forming a distinctive 'V-shape' with a hydrophobic cavity.[3] Their straight forward synthesis, unique cleft structure, and interesting photophysical properties have made TBNaps attractive for host- guest systems and various supramolecular assemblies.[4]We have developed multiple structures, materials, and polymers from TBNaps and demonstrated their potential uses. For example, a novel Tröger's base *p*-cymene-Ru(II)-curcumin organometallic conjugate was utilized as a theranostic agent against cervical cancer cells.[4]Recently, we created a TBNaps-functionalized triazine covalent organic polymer for 'turn-on' fluorescent detection of volatile organic pollutants.[5] In this presentation, I will elaborate on recent progress in supramolecular self- assembly and the creation of new structures and functional materials from TBNaps.



References:

1. Shanmugaraju S. Supramolecular Coordination Complexes: Design, Synthesis, and Applications. Elsevier Publications. 1st Edition, **2022**, Pages: 498, ISBN: 9780323907057.
2. Savyasachi, A. J.; Kotova, O.; Shanmugaraju, S.; Bradberry, S. J.; Maille, G. M.; Gunnlaugsson. T., *Chem*., **2017**, *3*, 764-811.
3. Shanmugaraju, S.; Dabadie, C.; Byrne, K.; Savyasachi, A. J.; Umadevi, D.; Schmitt, W.; Kitchen, J. A.; Gunnlaugsson, T., *Chem. Sci*., **2017**, *8*, 1535-1546.
4. Binduja, M.; Sandra E.-A.; Umadevi, D.; Poulsen, B. C.; Blasco, S.; McManus, G. J.;

Gunnlaugsson, T.; Shanmugaraju, S., *Inorg. Chem*., **2022**, *61*, 11592-11599.
5. Shanmughan, A.; Balamurugan, K.; Kalaiarasi, G.; Chitrarasu, K.; Shanmugaraju, S., *ACS Meas. Sci. Au*., **2025**, *5*, 56–62.

SHORT INVITED LECTURES

SIL 01

Two-pot and Single-pot Strategies for Hydroformylation-Aldol Condensation Based Synthesis of Jasminaldehyde over Heterogeneous Catalyst

N. Sudheesh[a,b], Ram S. Shukla[b]*

[a] *Department of Chemistry, N.S.S. College, K.R. Puram, Cherthala, Alappuzha, Kerala 688541, India*

[b] *Inorganic Materials and Catalysis Division, Council of Scientific and Industrial Research, Central Salt and Marine Chemicals Research Institute, G. B. Marg, Bhavnagar, Gujarat 364 002, India*

* *ramshukla55@yahoo.in*

Keywords: Jasminaldehyde, Aldol condensation, Hydroformylation, Heterogeneous catalyst

Jasminaldehyde is a perfumery chemical used for making floral notes. It was synthesized by base catalysed aldol condensation of heptanal and benzaldehyde.[1] Heptanal can be obtained by hydroformylation of hexene. In this study, a combined reaction of hydroformylation of hexene followed by aldol condensation of the product with benzaldehyde were perfomed in a two-pot and single-pot reaction methods. $HRh(CO)(PPh_3)_3$ encapsulated HMS was the hydroformylation catalyst and APTMS functionalised Chitosan was the aldol condensation catalyst. The catalysts were characterised with various techniques to confirm the encapsulation and functionalisation.[2,3] Two-pot synthesis gave 28% yield for jasminaldehyde in 36 h of reaction time. Single-pot synthesis gave 25% yield for jasminaldehyde in 16 h of reaction time.

References

1. Climent, M. J.; Corma, A.; Forne, V.; Guil-Lopez, R.; Iborra, S., *Adv. Synth. Catal.*, **2002**, *344*, 1090–1096.
2. Jos, T.; Sudheesh, N.; Shukla, R. S., *J. Mol.Catal. A: Chem.* **2010**, *333*, 158–166.
3. Sudheesh, N.; Sharma, S. K.; Shukla, R. S.; Jasra, R. V., *J. Mol.Catal. A: Chem.* **2008**, *296*, 61–70.

SIL 02

A Facile Biomimetic Potentiometric Sensor for Trace-Level Monitoring of Methyl Paraben

Saumya Varghese[a,*], Anjana Kolarveetil Rajagopalan[a], Sanjay Saji[a]

[a]*Department of chemistry, St. Joseph's college(autonomous), Devagiri, Calicut-673008, Kerala,India.Affiliated to University of Calicut*

**smyvp2000@gmail.com*

Keywords: Methyl paraben, Molecularly imprinted, Cosmetics, Potentiometric sensors.

Parabens (PBs) are esters of p-hydroxybenzoic acid, distinguished by various alkyl, aryl, or benzyl groups.[1] Among them, methylparaben (MPB) has been linked to adverse effects on women's reproductive health, including endometriosis, hormonal disruption, and elevated risks of uterine and ovarian cancers.[2,3] Methyl paraben (MP), a widely used preservative in pharmaceuticals, cosmetics, and food products, has raised growing environmental and health concerns due to its persistence and potential endocrine-disrupting effects, making its ultra-trace detection crucial for environmental monitoring and public safety. To the best of our knowledge, this work presents the first potentiometric sensor ever developed for methyl paraben, achieved through a biomimetic solid-contact design integrating low-tech potentiometry with molecular imprinting technology for highly selective, nanomolar-level detection. The MP-imprinted polymer, serving as the ionophore, was synthesized via Molecular Imprinting Technology (MIT) and characterized using FESEM and FTIR to confirm its morphology and template removal. The fabricated sensor operates effectively in the pH range 9.2–10.2, over a wide concentration range of 1×10^{-8} M to 1×10^{-4} M & 1×10^{-4} M to 1×10^{-2} M with respective slopes of -17.5 ± 0.17 mV and -55.8 ± 0.27 mV per decade with a limit of detection of 1×10^{-9} M. It demonstrates excellent sensitivity, selectivity, stability, and reusability, with a rapid response time of just 100 seconds. These characteristics render the sensor highly suitable for routine monitoring of methyl paraben in environmental water sources.

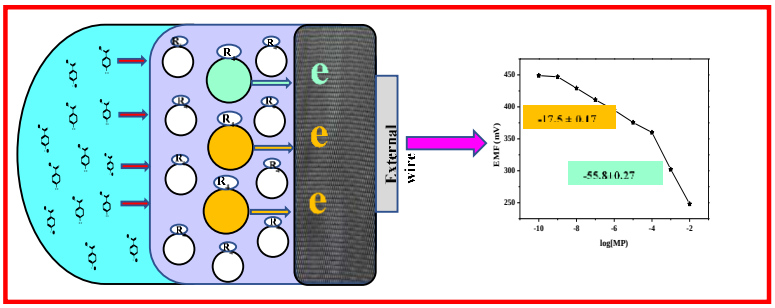


Figure 1: Graphical Representation of the developed biomimetic potentiometric methyl paraben sensor

References

1. Nguyen, D. M.; Toan, T. T. T., *ECS Sens. Plus* **2022**, *1*, 031603.
2. Xue, J.; Wu, Q.; Sakthivel, S.; Pavithran, P. V.; Vasukutty, J. R.; Kannan, K., *Environ. Res.* **2015**, *137*, 120.
3. Huo, W.; Xia, W.; Wu, C.; Zhu, Y.; Zhang, B.; Wan, Y.; Zhou, A.; Qian, Z.; Chen, Z.; Jiang, Y., *Environ. Pollut*. **2018**, *233*, 872.

SIL 03

Biomimetic Chemistry for Molecules to Materials: A Sustainable Way Forward for Dyestuff and Specialty Chemicals

Nabanita Sadhukhan[a,*], Swapnil Pawar, Rohit Ketkar, Viraj Sable, Ajinkya Rothe, Sanket Diwate, Harshal Barhate

[a]*Department of Specialty Chemicals Technology, Institute of Chemical Technology, Mumbai, Maharashtra – 400 019, India*

[*]*nn.sadhukhan@ictmumbai.edu.in, nnsadhukhan@gmail.com*

Keywords: Biomimetic catalysis, Oil epoxidation, Lotus effect mimicking, Self-cleaning cotton

Xanthene Oxidase is an enzyme known to catalyse various oxidation reactions, e.g., hypoxanthine to xanthine (Fig. 1A). The Molybdopterin cofactor is responsible for this oxidative transformation reaction. Alternatively, we synthesized a molybdenum-maltolate [MoO_2Mal_2] complex as a potential bio-mimicking catalyst that could emulate the natural enzyme xanthine oxidase (Fig. 1B). Furthermore, nature's existing "Lotus-leaf effect" has been a concept for creating super-hydrophobicity on material surfaces. Inspired by the same, the quest to create a lotus leaf effect on cotton fabric by dyeing was successfully achieved (Fig. 1C). Nature-driven molecular design, synthesis of bioinspired functional compounds and their application towards sustainable synthesis of commercially important molecules or materials will be discussed in the presentation.

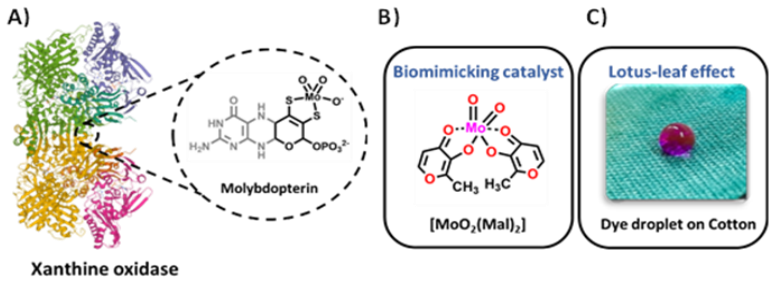


Figure 1. A) Xanthene Oxidase enzyme, B) [MoO_2Mal_2] catalyst works as a potential biomimetic catalyst, C) Lotus leaf effect was created on cotton by dyeing.

References

1. Pawar, S. S.; Ketkar, R. N.; Gaware, P. B.; Jagushte, K.U.; Dhawne, D.; Save, S. N.; Sharma, S.; Periyasamy, G.; Chimthanawala, N.; Sathaye, S.; Joshi, S.V.; Sadhukhan, N., *Dalton Trans.* **2024**, 53, 5770-5774.
2. Sadhukhan, N.; Diwate, S.; Rothe, A., *Indian Patent Application, 202521008854*

ORAL PRESENTATIONS

OP 01

Multi-Faceted *In Vitro* Bioactivity Assessments of a Diaminoguanidine Based Ligand and its Rare Manganese(II) Complex

Krishnapriya M. J.[a], Manoj E.[a,*]

[a] *Department of Applied Chemistry, CUSAT, Kochi, Kerala 682 022, India*

**manoje@cusat.ac.in*

Keywords: Diaminoguanidine, Anticancer, Antibacterial, Antidiabetic

The interconnected challenges of antimicrobial resistance, cancer, and diabetes highlight the urgent need for novel compounds that overcome resistance and selectively target diseased cells for effective therapy. Diaminoguanidine-based Schiff base ligands exhibit notable biological significance due to their flexibility and ability to interact with biomolecules, making them promising candidates for multifunctional therapeutic applications.[1,2] Here, we report the synthesis and physicochemical characterization of a diaminoguanidine based ligand, 1,3-bis(pyridin-4-ylmethylideneamino)guanidine hydrochloride ($H_3L{\cdot}HCl$), and its rare manganese(II) complex. Structural confirmation was achieved by single crystal X-ray diffraction, which validated the molecular geometry of both the ligand and the complex (Figure 1). The interesting aspect of the Mn(II) complex is the coordination of the ligands in protonated and cationic forms. DFT and MEP analyses of the complex provided insight into electronic properties and potential reactive sites. *In vitro* antibacterial activity of the Mn(II) complex was found to be better compared to the ligand. *In vitro* cytotoxicity studies on MCF-7 cells also demonstrated enhanced efficacy of complex with an IC_{50} value of 92.14 µM. Antioxidant investigations revealed IC_{50} values of 29.41 µM for the ligand and 25.69 µM for the complex, indicating considerable free radical scavenging potential. Additionally, both compounds displayed moderate antidiabetic activity.

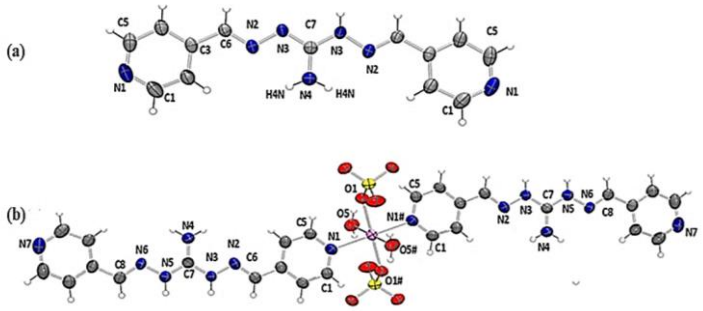


Figure 1. ORTEP diagram of (a) the ligand and (b) the complex**.**

References

1. Santu, A.; Hashim, K.K.M.; Manoj, E., *New J. Chem.* , **2024**, *48*, 4496–4506.
2. Hashim, K.K.M.; Manoj, E.; Kurup, M.R.P., *J. Mol. Struct.*, **2021**, *1246*, 131125.

OP 02

Development of Photo-Activable Ru (II)/Ir (III)-Benzodipyridophenazine Complexes for PDT: Synthesis, Characterization, Photophysical and Biological Studies

Nivedya T.[a], Ashok Kumar S.K.[a,*] and Priyankar Paira[a,*]

[a]*Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India.*

ashokkumar.sk@vit.ac.in, priyankar.paira@vit.ac.in

Keywords: Benzodipyridophenazine, DFT, Molecular docking, PDT, Hypoxia, GSH

The study investigated the impact of benzodipyridophenazine-based Ru (II) and Ir (III) complexes (**Ru1**, **Ru2**, **Ir1**, and **Ir2**) on their anticancer activity. Metal complexes displayed three significant absorption bands due to intra-ligand charge transfer (ILCT), ligand-to-ligand charge transfer (LLCT), and metal-to-ligand charge transfer (MLCT). *In vitro* screening identified that complex, **(Ir1)** exhibited the highest potency and selectivity (IC_{50} ~ 2.14 µM, PI > 13) under yellow light irradiation. Biomolecule binding tests using the complexes and ligand showed that attaching with Ru (II)/Ir (III) improved ligand characteristics. Chloro-substituted complexes (**Ir1, Ru1**) are effective for hypoxic tumour treatment, particularly **Ir1** which can generate high amounts of reactive oxygen species (ROS, Type I PDT) in cells under photo irradiation. Colocalisation study and DCFDA studies with **Ir1** revealed that it can accumulate in the mitochondria, leading to the depolarization of the mitochondrial membrane.

References

1. R. Das; P. Paira, *Dalton Trans.*, **2023**, *52*, 15365–15376.
2. S. De; R. Selva Kumar; A. Gauthaman; S. K. Ashok Kumar; P. Paira; A. Moorthy; S. Banerjee, *Inorganica Chim Acta,* **2021**, *515*, 120066.
3. H. R. Drew, R. E. Dickerson, *J Mol Biol*, **1981**, *151*, 535–556.

OP 03

Selective Detection of Al^{3+} by a Naphthyl Based Schiff Base in Water and Organic Solvent

Jinsha K C [a], Roymon Joseph [a,*]

[a]*Department of Chemistry, University of Calicut, Thenjipalam-673635, India*

**roy@uoc.ac.in*

Keywords: Schiff base, Aluminium, Fluorescence *turn-on*

Metal ions are known to play indispensable roles in numerous biochemical processes. Their concentration and distribution within body fluids have significant impact on the normal physiological function of the human body. Depending on their concentration, metal ions can either support biological functions or pose risks to human health and environment. Therefore, accurately identifying and quantifying metal ions has become a crucial focus in analytical science, leading to extensive research on the development of diverse metal ion sensing technologies.[1-2] In recent years, Schiff base ligands have garnered significant interest among researchers for metal ion detection, owing to their versatile structural features and broad spectrum of physicochemical properties. Consequently, these ligands have been investigated for a variety of potential applications across multiple scientific fields, particularly in medicine and pharmacology as antimicrobial, antifungal, and anticancer agents. They also act as catalysts in various organic reactions and play a crucial role in analytical chemistry for the detection of metal ions.[3-5] In the present study, amino derivative of 1,8-naphthalic anhydride was linked to a 2-hydroxy naphthaldehyde unit via an imine bond to obtain the Schiff base, **SB1**. The fluorescence spectroscopy revealed that **SB1** exhibits remarkable selectivity for Al^{3+} ions over 11 other metal ions. The detection of **SB1** by Al^{3+} has been monitored by a fluorescence *turn-on* mechanism with a fluorescence enhancement fold of ~ 4 and ~ 2 fold in water and in methanol respectively. The selectivity of **SB1** towards Al^{3+} in the presence of other metal ions was evaluated by competitive titration wherein Fe^{2+}, Fe^{3+}, Cu^{2+}, and Hg^{2+} exhibit marginal interferences in water while no interference was detected in methanol. The Job's plot analysis confirmed a 1:1 stoichiometric ratio between **SB1** and Al^{3+} in both solvents. The minimum concentrations of **SB1** required to detect Al^{3+} in a sample by fluorescence spectroscopy was found to be $1.7 \cdot 10^{-7}$ and $2.7 \cdot 10^{-7}$ M in water and methanol respectively. These observations were further supported by UV-visible and ^{1}H NMR spectroscopy.

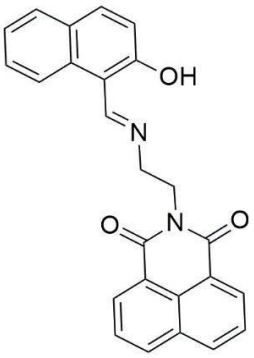


Figure 1. Structure of SB1.

References

1. Zoroddu, M. A.; Aaseth, J.; Crisponi, G.; Medici, S.; Peana, M.; Nurchi, V.M., *J. Inorg. Biochem.*, **2019**, *195*, 120–129.
2. Jomova. K.; Makova. M.; Alomar. S.Y.; Alwasel. S.H.; Nepovimova, E.; Kuca, K.; Rhodes, C.J.; Valko, M., *Chem. Biol. Interact*, **2022**, *367*, 110173.
3. Peng, H.; Han, Y.; Lin, N.; Liu, H., *Opt. Mater.* **2019**, *95*, 109210.
4. Hoque, A.; Islam, M. S.; Khan, S.; Datta, B.; Zangrando, E.; Kole, G. K.; Alam, M., *Dalton Trans.* ,**2023**, *52*, 10145-10154.
5. Tian, J.; Yan, X.; Yang, H.; Tian, F., *RSC Adv.*, **2015**, *5*, 107012-107019.

OP 04

In Situ Synthesized MoS_2 Scaffolded $CsPbBr_3$ Hybrids: Probing Interfacial Charge Transfer Dynamics

Linda Maria Varghese[a], Fency Sunny[b], Gaurav Jhaa[c], Sam John[d], Nandakumar Kalarikkal[b,e] , Priyakumari Chakkingal Parambil[c], Kurukkal Balakrishnan Subila[a,f,*]

[a]*School of Chemical Sciences, Mahatma Gandhi University, Kottayam 686 560, Kerala, India.*

[b]*International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam 686 560, Kerala, India.*

[c]*Department of Chemical Sciences, Indian Institute of Science Education and Research Mohali, India.*

[d]*Department of Chemistry, St. Berchmans College (Autonomous), Mahatma Gandhi University, Kottayam, India.*

[e]*International Centre for Ultrafast Studies, Mahatma Gandhi University, Kottayam, Kerala, India.*

[f]*Advanced Molecular Material Research Centre, Mahatma Gandhi University, Kottayam, India.*

[a,f*] *subila@mgu.ac.in*

Keywords: $CsPbBr_3/MoS_2$ hybrid, In situ synthesis, Charge transfer

The inorganic perovskite $CsPbBr_3$ distinguishes itself with exceptional optical characteristics, boasting a high quantum yield, robust light absorption, heightened luminous efficiency, and an adjustable luminous wavelength[1]. These qualities uniquely position $CsPbBr_3$ for significant applications across various fields. However, perovskite material facing the problem of instability and which can be improved by incorporating 2D materials like Molybdenum sulfide (MoS_2).[2]

In this study we explore the temperature-dependent phase transformation MoS_2 and the hybrid formation of $CsPbBr_3/MoS_2$. MoS_2 scaffolded $CsPbBr_3$ hybrid were synthesised by insitu method, enabling perovskite nucleation directly on the MoS_2 surface. Its morphology from FESEM analysis, TEM and EDS analysis and Elemental mapping further substantiates the success of integrating perovskite uniformly into the exfoliated MoS_2. The charge transfer between them is well studied through absorption studies, steady state photoluminescence studies and Life time analysis. Femtosecond transient absorption (fs-TA) spectroscopy revealed ultrafast charge transfer in the hybrids and an electron transfer rate of 4.30×10^{10} s^{-1} for $CsPbBr_3$@1T/2H-MoS_2. Charge transfer was further explained through electrochemical studies and from Mott Schottky analysis mechanism of charge transfer is predicted as quasi type II mechanism. DFT calculations reveal stronger stabilization for the $PbBr_2$-terminated $CsPbBr_3$ from enhanced orbital overlap and van der Waals interactions. Phase and interface engineering in perovskite - MoS_2 hybrids

enhances charge separation, enabling superior optoelectronic and photocatalytic applications.

References

1. Wang, Z.; Mi, B., *Environ. Sci. Technol*. **2017**, 51, 8229 - 8244.
2. Barua, S.; Dutta, H. S.; Gogoi, S.; Devi, R.; Khan, R., *ACS Appl. Nano Mater*, **2017**, 1, 2 - 25.

OP 05

Insight into the Crystal Structure and Optical Response of Cation Modulated Cs_2MCl_6 (M=Sn and Te) Vacancy Ordered Halide Perovskites

Nima A. M.[a], Subodh Ganesanpotti[a,*]
[a]*Department of Physics University of Kerala*
[*]*gsubodh@gmail.com, gsubodh@keralauniversity.ac.in*

Keywords: Solvothermal method, Vacancy ordered halide perovskites, Self trapped excitons, Density functional theory.

Lead halide perovskite has aroused a great attention in optoelectronic as well as photovoltaic applications because of their unique properties like high photoluminescence quantum yield, wide color gamut and tunable emission. However, their widespread use is limited due to the toxicity and instability associated with lead. These challenges can be resolved by developing lead free alternatives and substitution strategies to improve the safety and stability of perovskite materials. One such strategy involves replacing two Pb^{2+} ions with a single tetravalent cation such as Sn^{4+} or Te^{4+}, resulting in a defect perovskite variant known as vacancy ordered halide perovskites (VOHP) with the general formula A_2BX_6.[1] This work aims to investigate how variation in B-site cations (Sn/Te) influences the structural and optical properties of VOHPs.

We developed a facile solvothermal method to synthesis highly stable and efficient Cs_2MCl_6 (M=Sn and Te) VOHP. The crystal structure identification and phase purity confirmation of the synthesised compounds were done by using XRD, Raman and FTIR. Detailed morphological studies were performed using HRTEM, and the results were correlated with the crystal structure analysed by XRD. The synthesised materials exhibit enhanced thermal stability, as confirmed by thermogravimetric analysis and temperature-dependent Raman spectroscopy. The materials retain a similar crystal structure even when the B-site cation is varied. However, Sn-based compounds are non-emissive, whereas Te-based compounds exhibit strong photoluminescence. The variations in optical properties arise from changes in the band structure, as explained by density functional theory (DFT) analysis. The broad yellow emission of Te based compound is originating from the recombination of self-trapped excitons (STEs), as confirmed by lifetime analysis, and the detailed photoluminescence mechanism has been elucidated.[2] The emission of Te based compounds further highlights its potential for application in the fabrication of white LEDs.

References

1. Jiang, J.; Niu, G.; Sui, L.; Wang, X.; Zeng, X.; Zhang, Y.; Yang, X., *Adv. Opt. Mater.*, **2023**, *11*, 2202634.
2. Xu, Z.; Jiang, X.; Cai, H. P.; Chen, K.; Yao, X.; Feng, Y., *J. Phys. Chem. Lett.* **2021**, *12*, 10472-10478.

OP 06

Thermodynamic and Kinetic Study on Adsorption of Cu (II) Using Multi-functionalised Organo Clay

Sneha S[a], Anjali R Mohan [a], Bency John [a,*]
[a]*Department of chemistry, SG College Kottarakara, Kollam - 691531, Kerala, India*
[*]*bencyjohn136@gmail.com*

Keywords: Montmorillonite clay, Adsorbent, Characterization, Adsorption kinetics, Cu (II) removal

In the present work, a surfactant-modified organoclay was synthesized and used as an efficient adsorbent for the removal of Cu(II) ions from aqueous solution. Sodium montmorillonite (Na-MMT) was chosen as the base clay and modified with the cationic surfactant cetyltrimethylammonium bromide (CTAB) and humic acid (HA). The modification was confirmed through FTIR, SEM, TGA, XRD, and BET analyses, which revealed enhanced surface properties and increased surface area. Batch adsorption experiments were conducted to investigate the effects of pH, contact time, temperature, and initial metal ion concentration. Maximum adsorption efficiency of 83.33% was observed at pH 6 and an initial Cu(II) concentration of 50 mg/L [1]. Equilibrium data were best described by the Freundlich isotherm model (R^2 = 0.9904), suggesting multilayer adsorption on a heterogeneous surface, whereas the Langmuir model (R^2 = 0.9849) showed slightly lower correlation [2]. Kinetic studies indicated that the pseudo-second-order model (R^2 = 0.9267) provided the best fit, implying chemisorption as the rate-controlling step [3]. Thermodynamic analysis revealed that Cu (II) adsorption was spontaneous and endothermic, with $\Delta H°$ = 87.14 kJ/mol and $\Delta S°$ = 286.28 J/K·mol, indicating increased randomness at the solid–liquid interface. Overall, Cu (II) removal using CTAB/HA-modified Na-MMT was efficient, sustainable, and eco-friendly, demonstrating the organoclay's potential as a superior adsorbent for heavy metal remediation.

References

1. Lamrani, M.; Mouchane, M.; Taybi, H.; Mouadili, A., *J. Water Environ. Nanotechnol.*, **2025,** *10*, 85-107.
2. Ahmad, R.; Mirza, A., *Groundw. Sustain. Dev.*, **2017,** *4*, 57-65.
3. Haounati, R.; Ouachtak, H.; El Haouti, R.; Akhouairi, S.; Largo, F.; Akbal, F.; Addi, A. A., *Sep. Purif.Technol.*, **2021,** *255*, 117335.

OP 07

2D CuO Thin Films via Spray Pyrolysis for Glucose Sensing

Anaswara J. S.[a], R. Jayakrishnan[a,*]

[a]*Photovoltaic Research Laboratory, Department. of Physics, University of Kerala, Kariyavattom, 695581, India*

[*]*rjk@keralauniversity.ac.in*

Keywords: Copper Oxide (CuO), Thin films, Spray Pyrolysis

Copper oxide (CuO) exhibits notable sensitivity and catalytic activity, making it a promising candidate for sensing applications. However, its practical deployment is often constrained by key challenges such as elevated operating temperatures, limited analyte selectivity, insufficient detection limits and concerns over long-term material stability.[1, 2] To overcome these limitations, we focus on engineering high-performance CuO thin films through the spray pyrolysis technique. This method offers a cost-effective and scalable approach for thin film fabrication, wherein a precursor solution is atomized and deposited onto a heated substrate, triggering thermal decomposition and forming the desired material. Spray pyrolysis is particularly advantageous for producing highly stable, uniform thin films across large surface areas. Previous studies that explored non-enzymatic glucose sensing using CuO thin films deposited by spray pyrolysis, found that film thickness significantly affected the sensitivity due to changes in conductivity and surface roughness.[1, 2, 3] In the present work we optimize the spray pyrolysis process to grow nano-crystalline thin films and functionalize the thin films to demonstrate their glucose sensing capability.[4] Structural characterization of the grown thin films using X-ray diffraction studies show that the deposition of monoclinic CuO phase was achieved with our process temperature of 573 K. The average crystallize size of the grown thin films was found to be 10 nm. The optical bandgap of the 2D CuO thin films was found to be 1.5 eV using the Tauc plot. Glucose sensing is demonstrated and analyzed using cyclic voltammetry. The 2D CuO-based sensors grown by us show distinct redox peaks when glucose is present, allowing for its quantification while the peak current response correlates with glucose concentration, which enables the determination of the sensor's sensitivity.

References

1. Ghosh, A.; Schneller, T.; Waser, R.; Majumder, S. B., *Sens. Actuators B Chem.*, **2017**, *253*, 685-696.
2. Xiang Peng; Jiabei Liu; Yuming Tan; Rong Mo; Yong Zhang, *Sens. Actuators B Chem.*, **2022**, *362 131775*.
3. Cory N. J.; Visser, E.; Chamier, J.; Jessica Chamier; Juliet Sackey; Franscious Cummings; Mahabubur Chowdhury, *Appl. Surf. Sci.*, **2022,** *576*, 151822.

4. A.Moumen; B.Hartiti; E. Comini ; Z. Elkhalidi; H.M.M.Munasinghe Arachchige; S.Fadili; P.Thevenin, *Superlattices and Microstructures*, **2019**, *127*, 2-10.

OP 08

MXene-Accelerated Hierarchical Assembly of Ce-MnO_2/PEDOT Nanohybrids at Liquid/Liquid Interface for Electrochemical Sensing Application

Anjali S[a], Mini Mol Menamparambath[a,*]
[a] *Department of Chemistry, National Institute of Technology Calicut, Kerala, India*
[*] *minimol@nitc.ac.in*

Keywords: $Ti_3C_2T_x$ MXene, Ce-doped MnO_2/PEDOT nanohybrid, L/L Interface, Electrochemical sensing.

In the rapidly advancing field of functional nanomaterials, the bisolvent interface between immiscible liquids has emerged as a powerful platform for constructing structurally tailored nanohybrids. This energetically active boundary enables directed polymerization and the formation of integrated hybrids with tunable architectures and enhanced properties.[1,2] MXenes offer metallic conductivity, tunable surface terminations, and high structural adaptability, marking them as transformative materials in this context.[3,4] Although widely explored in energy storage, catalysis, and sensing, their role in steering interfacial polymerization remains largely untapped. Here, $Ti_3C_2T_x$ MXene serves as a conductive template to drive and accelerate the interfacial oxidative polymerization of EDOT, yielding MXene-based Ce-doped MnO_2/PEDOT nanohybrid with strong structural cohesion and electronic continuity. Conducted at a chloroform/water interface using $KMnO_4$ and $Ce(SO_4)_2 \cdot 4H_2O$ as dual oxidants, the reaction proceeds six times faster upon MXene incorporation. This acceleration arises from the synergy of MXene's Bronsted-Lewis acidic sites and high conductivity, which collectively modulate interfacial redox kinetics and guide the orderly polymer growth, while simultaneously directing hybrid assembly and reinforcing the layered framework.[5] The MCMP nanohybrid, confined at the bisolvent interface, exhibits hierarchically ordered structure, uniform morphology, and integrated electron-transport networks, as confirmed by physico-chemical characterizations. When applied to carbon cloth yarn electrodes, the hybrid demonstrates improved electrochemical activity and high sensitivity toward metronidazole (MDZ), with rapid response and reliable performance in real-sample detection. This study highlights MXene not only as a structural scaffold but also as a mediator that directs interfacial redox dynamics and polymer growth, establishing a single-step, ambient strategy for constructing robust hybrid systems for sustainable sensing and energy applications.

References

1. Chondath, S. K.; Menamparambath, M. M., *Nanoscale Adv.*, **2021**, *3*, 918–941.

2. Sugunan, A.; Syamala, A. A.; Radhakrishnan, A. B.; Menamparambath, M. M., *Nanoscale Adv.*, **2025**, *7*, 4980–4993.
3. Gogotsi, Y.; Anasori, B., *ACS Nano*, **2019**, *13*, 8491–8494.
5. Wu, X.; Ma, P.; Sun, Y.; Du, F.; Song, D.; Xu, G., *Electroanalysis*, **2021**, *33*, 1827–1851.
6. Fei, X.; Wang, Y.; Guo, P.; Wang, J.; Wang, G.; Lu, G.; Zhao, W., *Ind. Eng. Chem. Res.*, **2024**, *63*, 6868–6879.

OP 09

Two-Electron Water Oxidation by Vanadium–Oxo Porphyrins through Electro- and Photoelectrocatalytic Pathways

Arifa Kaniyantavida[a], Jayachandran Kaippully[a], Haritha Anamangattupurakkal[a], Aparna chencharodi[a], Sebastian Nybin Remello[b], Hiroshi Tachibana[c], Haruo Inoue[c] and Fazalurahman Kuttassery[a*]

[a] *Department of Chemistry, University of Calicut, Malappuram 673635, Kerala, INDIA*
[b]*Department of Applied Chemistry, Cochin University of Science and Technology, Kochi 682022, Kerala, INDIA*
[c]*Department of Applied Chemistry for Environment, Graduate School of Urban Environmental Sciences, Tokyo Metropolitan University, 1 – 1 Minami Osawa, Hachioji, Tokyo 192 – 0397, JAPAN*
[*] *kfazalurahman@uoc.ac.in*

Keywords: Photoelectrochemical system, Molecular catalysis, Two electron water oxidation

Artificial photosynthesis offers a promising route toward sustainable fuel production. Since the discovery of the "blue dimer," bio-inspired molecular catalysts have attracted considerable attention for water oxidation. However, the conventional four-electron oxygen evolution reaction (OER) is intrinsically sluggish due to the need to accumulate multiple redox equivalents.[1] Here, we report vanadium–oxo porphyrin complexes that promote an alternative and more kinetically favorable two-electron water-oxidation pathway. Neutral (VOTPyP) and cationic (VOTMPyP) porphyrins were synthesized and electrochemically benchmarked. The cationic complex VOTMPyP exhibited superior electrocatalytic performance, achieving current densities up to 1.5 mA cm^{-2} at 1.36 V vs. SHE under homogeneous conditions. Controlled-potential electrolysis at pH 12.5 revealed H_2O_2 as the primary oxidation product with a Faradaic efficiency of up to 93.6%. To explore photo-electrocatalytic behavior, hybrid molecular–semiconductor electrodes were constructed by anchoring neutral VOTPyP or anionic VTCPP onto TiO_2 and SnO_2 films. The VOTPyP/SnO_2 photoanode delivered nearly two orders of magnitude higher photocurrent than VOTPyP/TiO_2 and achieved an APCE of 16% in pure water without sacrificial donors. These results identify vanadium–oxo porphyrins as efficient molecular platforms for selective two-electron water oxidation and highlight the VOTPyP/SnO_2 hybrid as a promising photoanode for integrated artificial Z - Scheme systems by coupling with CO_2 reduction photocathodes. [2]

References

1. F. Kuttassery; S. Mathew; S. N. Remello; A. Thomas; K. Sano; Y. Ohsaki; Y. Nabetani; H. Tachibana; H. Inoue, *Coord. Chem. Rev*., **2018**, *377*, 64-72.
2. F. Kuttassery; Y. Ohsaki; A. Thomas; R. Kamata; Y. Ebato; H. Kumagai; R. Nakazato; A. Sebastian; S. Mathew; H. Tachibana; O. Ishitani; H. Inoue, *Angew. Chem. Int. Ed*., **2023**, *62*, e202308956.

OP 10

Computational Insights into Structural, Electronic and Optical Properties of Cs_2BCl_6 (B = W, Mo)

Lekshmi M. D.[a], Subodh G[a], Jawahar I N[a,*]

[a]*Department of Physics, University of Kerala, Thiruvananthapuram, Kerala*

[*]*jawaharin_4929@keralauniversity.ac.in*

Keywords: Density functional theory, Generalized gradient approximation, Ultrasoft pseudopotential.

The perovskite family (ABX_3) is known for its structural flexibility and compositional tunability. The search for non-toxic and stable alternatives to lead-based perovskites has led to growing interest in lead-free halide perovskites[1,2]. In this study, we investigate the structural, electronic, and optical properties of a lead-free halide perovskite, Cs_2BCl_6 (B = W, Mo), which belongs to the class of vacancy-ordered double perovskites with the general formula A_2BX_6, using first-principles calculations based on density functional theory (DFT). The calculations are performed using the CASTEP module in Materials Studio, and the structure is optimized using the Generalized Gradient Approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) functional. Ultrasoft pseudopotential is employed to ensure computational efficiency and accuracy. Electronic structure calculations, including spin–orbit coupling (SOC) and DFT+U corrections to account for the partially filled d-orbitals, reveal a suitable band gap, suggesting potential for optoelectronic applications[3,4]. A comparative analysis of different B-site elements revealed profound insights into how subtle compositional changes can finely tune the properties of both materials, highlighting the potential for targeted property optimization.

References

1. Li, T., *Phys. Rev. Appl.*, **2018,** *10*.
2. Ghorui, S., *Phys. Rev. Appl.*, **2024**, *21*.
3. Hossain, M. N.; Anwar Hossain, M.; Hossain, M. M., *Phys. Scr.*, **2025**, *100*, 125807.
4. Bhatti, A. S.; Choudhury, M. A.; Hussain, S., *J. Phys. Chem. C*, **2025**, *129*, 24012.

OP 11

Carboxylic Acid-Functionalized β-Keto Enamine-Linked Porous Organic Polymer Based Fluorescent Immuno Assay for Prostate Cancer Detection

Sreelakshmi T. Prasad[a], Kala R[a,b]*

[a] *Department of Applied Chemistry, Cochin University of Science and Technology, Kochi 682022 India*

[b]*Inter University Centre for Nanomaterials and Devices, Cochin University of Science and Technology, Kochi 682022 India*

**kala@cusat.ac.in*

Keywords: Fluorescent Immuno assay, Prostrate specific antigen, Porous organic polymer, β-Ketoenamine linkage.

Prostate-specific antigen (PSA) is a crucial biomarker for the early diagnosis and monitoring of prostate cancer, one of the leading causes of cancer-related deaths among meworldwide[1]. Conventional immunoassays for PSA detection, though accurate, often require sophisticated instrumentation, skilled personnel, and lengthy processing times, limiting their suitability for rapid clinical screening. In this context, fluorescence-based immunoassays have gained significant attention due to their high sensitivity, simplicity, and potential for point-of-care diagnostics. The development of cost-effective, and highly selective fluorescent probes for PSA detection is therefore of great importance in improving early disease diagnosis and patient management.

In this work, we have developed a fluorescent immunosensing platform based on a carboxy-functionalized porous organic polymer, DHBTC–DAB, conjugated with PSA antibody via EDC coupling chemistry. The resulting DHBTC–DAB Ab conjugate exhibited excellent photostability, selectivity, rapid response and sensitivity toward PSA, with a distinct fluorescence quenching response upon antigen binding. Compared to reported systems, this conjugate demonstrates superior performance and strong potential for real-time and point-of-care PSA detection.

References

1. Msutu, T.; Adeniyi, O., *Sens. Diagn.* **2024**, *3*, 1167-1176.

OP 12

Unveiling Surface Binding of Polymeric Substrate in Enzyme Catalysis: Insights from PET Hydrolases

I. V. Krishnendu[a], Susmita De[a,*]
[a]*Department of Chemistry, University of Calicut, Malappuram, India*
[*]*susmita@uoc.ac.in*

Keywords: PET hydrolases, Enzyme catalysis, Surface binding sites

Plastic biodegradation provides an environmentally benign approach for plastic waste valorization and recycling.[1] PET hydrolases degrade PET, a strong, recyclable, and chemically resistant polymer.[1] Enzyme–substrate complex formation, a critical step in catalysis, determines the specificity and selectivity of the reaction,[2] which even becomes particularly significant in the case of polymeric PET which can interact with multiple sites on the protein surface simultaneously. Although catalytic sites are crucial for activity, mutations at both catalytic and non-catalytic sites in PETases have been found to alter catalytic efficiency.[3] This work explores specificity of substrate binding in wild-type and mutated PET hydrolases using molecular dynamics simulations. Our results revealed additional competitive sites that may interfere with selective binding at the active site, thereby reducing catalytic efficiency (Figure 1). This suggests that regulating non-catalytic binding could improve catalytic performance by enhancing substrate selectivity toward the catalytic site.

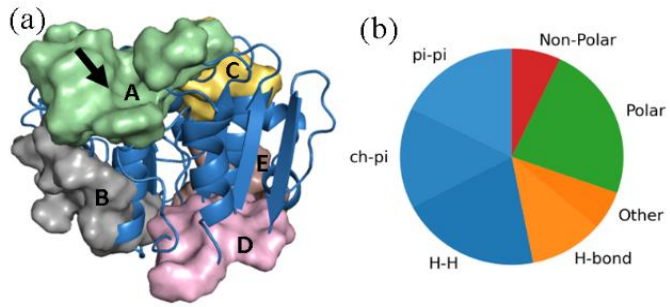


Figure 1(a) Surface binding sites on *Is*PETase depicted as coloured surface representations: Site A (green), Site B (grey), Site C (yellow), Site D (pink), and Site E (brown). The catalytic site is indicated with a black arrow. **(b)** Binding energy decomposition pie chart of catalytic site A indicating types of interactions.

References

1. Tournier, V.; Duquesne, S.; Guillamot, F., *Chem. Rev.*, **2023,** *123*, 5612−5701.
2. Palmer,T; Bonner ,P.L, *Enzymes: Biochemistry, Biotechnology, Clinical Chemistry (2nd ed.).*, **2019,** Woodhead Publishing.
3. James, A.; De,S., *RC Adv.*, **2022**, *12*, 20563.

OP 13

Eco-Friendly Carbon Dots from *Pistia stratiotes L.*: Development of a Biodegradable Sensor for Selective Detection of Levofloxacin in Water

Jaisy Joy[a,b,c], Annu Thomas[b,c*], Beena Mathew[a,*]

[a] *School of Chemical Sciences, Mahatma Gandhi University, Priyadarsini Hills P.O., Kottayam, 686 560, Kerala, India.*

[b] *Research and Postgraduate Department of Chemistry, Kuriakose Elias College, Mannanam P.O., Kottayam 686561, Kerala, India.*

[c] *Department of Chemistry, Bishop Chulaparambil Memorial College, Kottayam 686001, Kerala, India.*

[*] *beenamathew@mgu.ac.in, [*] annuthomas@bcmcollege.ac.in*

Keywords: Carbon dots, Polyvinyl alcohol, Polymer-composite film, Levofloxacin, Fluorescence sensing.

Carbon dots (CDs), recognised for their stable and tunable emission properties, have gained momentum as eco-friendly fluorescent probes. This study presents a cost-effective method for synthesising CDs from the aquatic plant *Pistia stratiotes L.*[1]The morphological, optical, and structural analyses of the CDs revealed that they have an average diameter of 2.67 nm and emit strong blue fluorescence with excitation and emission maxima at 375 nm and 455 nm, respectively, alongside an absolute quantum yield of 7.52%. Their surface is rich in hydroxyl, carbonyl, and amino groups, with a negative zeta potential of -16.2 mV. The CDs serve as highly sensitive and selective sensors for detecting the antibiotic levofloxacin (LFN) in water and demonstrate high stability and excellent solubility. The detection mechanism is rapid, with optimal performance at pH 4 and a limit of detection (LOD) of 0.799 μM. A biodegradable polymer composite film (PVA-CA-CDs) incorporating the CDs in polyvinyl alcohol (PVA) matrix was also developed, maintaining strong fluorescence and stability, detecting LFN in micro volumes (20 μL) with an LOD of 7.16 μM.[2] TEM, FE-SEM, and atomic force microscopy (AFM) confirmed uniform dispersion of CDs within the polymer matrix. Validated through analyses of real water samples, recovery values ranged from 95% to 102%, observed for both solution-phase and solid-state sensors. This research is the first to use CDs from *Pistia stratiotes L.* for LFN detection and introduces an environmentally friendly polymer composite for this purpose.

References

1. Mathew, S. *et al. Mol. Struct.*, **2023**, *1294*, 136422.
2. Joy, J.; Thomas, A.; Mathew, B., *J. Fluoresc.*, **2025**, *18*, 1–21.

OP 14

N-doped Holey Graphene-Based Wires for Flexible Electronics

Haritha Valiyaveettil Padi[a], Binitha N. Narayanan [a,b,*]

[a]*Department of Chemistry, University of Calicut, Thenhipalam, Kerala, Calicut University, India*

[b]*Inter University Centre for Hydrogen & Energy Storage, University of Calicut, Thenhipalam, Kerala, Calicut University, India*

[*]*binithann@yahoo.co.in*

Keywords: Coin cell supercapacitor, Conducting ink, Graphene amine, Holey graphene, N-doping

Flexible conducting materials are essential for next-generation wearable and bendable electronic devices. In this study, we report a facile synthesis of N-doped holey graphene and its use as a promising flexible conducting wire. The material was obtained through a simple ball-milling of graphite followed by high-temperature treatment with an Nitrogen containing milling agent. Structural and morphological analyses, using TEM, XPS, XRD, FESEM, FTIR spectroscopy, Raman spectroscopy, ^{13}C NMR spectroscopy, and elemental analysis, confirmed the successful formation of the N-doped holey graphene structure with well-developed porosity and nitrogen incorporation in various forms. The interconnected and porous network structure facilitates efficient charge transport, while nitrogen doping enhances electrical conductivity and chemical stability. Graphene inks prepared and cured at various temperatures, including room temperature, exhibited tunable conductivity, demonstrating the potential of N-doped holey graphene as a promising material for flexible electronic wiring and printable circuit applications.

References

1. Htwe, Y. Z. N. et al. *J. Sci. Adv. Mater. Devices* **2022**, *7*, 100435.
2. Wei, D. et al. *Nanotechnology* **2011**, *22* , 245702.
3. Lai, L. et al. *Carbon* **2011**, *49* , 3250–3257.
4. Caliman, C. C. et al. *RSC Adv.* **2018**, *8* , 6136–6145.

OP 15

Boosting the CO_2 Reduction Activity of Cu Double Atom Catalyst through Coordination Environment Engineering

Seerat Amin,[a,b,] Manzoor Ahmad Dar[c,*], Sailaja Krishnamurty[a,b,*]

[a]*Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory (CSIR-NCL), Pune 411008, India.*

[b]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad – 201002, India*

[c]*Department of Chemistry, Islamic University of Science and Technology, Awantipora, Jammu and Kashmir-192122, India*

[a,b*]*sailaja.raaj@gmail.com*,[c*]*manzoor.dar@islamicuniversity.edu.in*

Keywords: Density functional Theory, CO_2RR, Cu_2-DACs, Coordination environment engineering.

Double-atom catalysts (DACs) offer a reasonable and scalable route towards carbon neutrality owing to their efficient catalytic features. However, the challenges associated with the flexibility of their coordination structure usually restrict their full potential as efficient catalysts. Herein, we comprehensively examined the impact of coordination environment regulation on the CO_2R activity of Cu_2-DACs supported on C, N, or B co-doped graphene using ab initio simulations. We highlighted the marked role of the local coordination sphere of Cu_2-DACs in modulating their structural stability and charge transfer characteristics, thereby regulating the adsorption of CO_2 and various reaction characteristics. Boron and carbon-coordinated Cu_2 centers (Cu_2–BxCy) exhibit strong CO_2 adsorption (-0.65 to -2.31 eV) due to enhanced electronic interactions, whereas carbon-nitrogen and nitrogen-boron coordination (Cu_2–NxCy, Cu_2–NxBy) led to weaker binding, underscoring the coordination environment's key role in CO_2 activation. The varying CO_2 interactions in these systems were further comprehended and supported by a multilevel descriptor (€) combining both geometric and electronic parameters. Moreover, the dynamic behaviour in the adsorption modes led to partial breakdown of the conventional linear scaling relations between the key CO_2 reduction intermediates (*COOH, *CO, and *HCO). Among the numerous types of investigated electrocatalysts, Cu_2-B_5C_1 emerged as a highly active and selective catalyst for methanol production, with a remarkably low limiting potential of -0.54 V, surpassing the performance of several reported Cu-based systems. Besides, our findings underscored the often-overlooked yet crucial role of explicit solvation, which significantly altered both the potential-determining step and product selectivity. These outcomes emphasized the necessity of including solvation effects in realistic electrochemical modelling. Collectively, this study provides a critical mechanistic insight into better understanding the coordination effect on the CO_2R and a robust design strategy for next-generation Cu-

based DACs, guiding the development of highly efficient and selective catalysts for CO_2 electroreduction.

References

1. Sun, H.; Liu, J.-Y., *ACS Catalysis*, **2024**, *14*, 14021-14030.
2. Ma, M.; Seger, B., *Angew. Chem. Int. Ed.*, **2024**, *63*, e202401185.

OP 16

A Facile, Sustainable and Efficient Polymer-Supported Nickel Catalyst for Alkyne–Azide Cycloaddition in Water

Arya Suku[a], Riya Raj[a], Praveena A P[a], Saithalavi Anas[a,b,*]

[a]*School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala, India-686560*

[b]*Advanced Molecular Materials Research Centre, Mahatma Gandhi University, Kottayam, Kerala, India-686560*

**anas@mgu.ac.in*

Keywords: Click reaction, Polymer support, Green Chemistry, Heterogeneous catalyst

Click chemistry, first introduced by K. Barry Sharpless and co-workers, has emerged as a powerful concept in modern synthetic chemistry due to its atom economy, operational simplicity, and high efficiency. Classical click involves regioselective cycloaddition between an organic azide and alkyne to generate 1,4 disubstituted 1,2,3 triazole product in presence of copper catalyst.[1] Although copper is the most widely used catalyst in click chemistry, alternative non precious metals have also been attracted increasing attention. Among them, nickel is an important sustainable, earth-abundant, and cost-effective alternative. Despite its potential, nickel-catalysed azide–alkyne cycloaddition (NiAAC) reactions remain relatively underexplored, with only limited studies reported. Most documented systems predominantly yield 1,4-disubstituted 1,2,3-triazoles while only a few produce 1,5-disubstituted triazoles as the major products, often accompanied by minor amounts of the 1,4-isomer.[2] Therefore, achieving regioselective click reaction leading to 1,5-disubstituted triazoles using nickel catalysts remains a significant challenge. To date, significant advancements have been achieved in heterogeneous catalysed click reactions to overcome the limitations associated with their homogeneous system. Recently our group have developed a number of modified PAN supported heterogeneous catalytic systems for diverse organic reactions[3,4] including click reaction.[5]

In this work, we report the development of a novel monoethanolamine-functionalized polyacrylonitrile-supported nickel catalyst (**mPAN–Ni**) for click reaction. This catalyst offered sustainable, regioselective synthesis of 1,5-disubstituted 1,2,3-triazoles via a one-pot, three-component reaction of alkyl halide, sodium azide, and alkyne in water and found to be general over various substrates (Scheme. 1) This approach provides a greener and environmentally benign alternative for triazole synthesis while maintaining high selectivity and efficiency.

Scheme 1: Schematic representation of AAC using mPAN-Ni

References

1. Kolb, H. C.; Finn, M. G.; Sharpless, K. B., *Angew. Chem. Int. Ed.* **2001**, *40*, *2004*.
2. Aslaheh, H. S.; Payamifar, S.; Marjani, A. P., *Appl. Organomet. Chem*. **2024**, *38*, *e7692.*
3. Sruthi, P. R.; Roopak, R.; Anas, S., *ChemistrySelect* **2023**, *8*, *e202204374*.
4. Sruthi, P. R.; Anas, S., Indian Patent No.391 643 *granted on* **10.03.2022.**
5. Arya, S.; Asiya, A. S.; Anas, S., *New J. Chem*. **2024**, *48*, *17385.*

OP 17

Structural Insights into the Reactant and Intermediate States of Enzyme Catalyzed PET Degradation

Muhasina P. V.[a], Susmita De[a,*]

[a]*Department of Chemistry, University of Calicut, Calicut University P.O., Malappuram 673 635, Kerala, India*

[*]*susmita@uoc.ac.in*

Keywords: PET hydrolases, Acylation, MD simulation, Binding energy.

Enzymatic biodegradation of polyethylene terephthalate (PET) seeks efficient enzymes with high catalytic activity and robust thermostability traits.[1] Several PET hydrolases with improved activity have been developed through targeted mutations and other structure-guided strategies based on conformational studies and PET binding analyses.[1] Theoretical investigations have revealed that PET hydrolysis proceeds *via* an acylation - deacylation mechanism involving multiple enzyme-substrate intermediates.[2] Since overall catalytic efficiency depends not only on substrate binding but also on the stability of intermediates and the efficiency of product release, elucidating the structural features and energetics of these intermediates and the associated transition states is essential. Here, we present a structure-based systematic analysis of the acylation step in the enzyme *Ca*PETase using molecular dynamics (MD) simulations and quantum mechanical (QM) calculations.[3] The MD analysis and MM/GBSA binding energy calculations of *Ca*PETase-PET complexes in the reactant (**R**) and tetrahedral intermediate (**Td-Int**) states reveal the involvement of distinct residues in stabilizing each state, along with aromatic and hydrophobic residues that contribute in both cases (Figure 1).

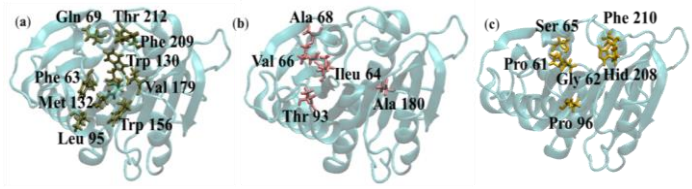


Figure 1. Important residues involved in the stabilization of (a) both reactant (**R**) and Intermediate (**Td-Int**) state (b). Reactant (**R**) and (c) Intermediate (**Td-Int**) in the first step of acylation in *Ca*PETase. Cartoon representation of *Ca*PETase is shown in cyan colour.

References

1. Veluru, S.; Seeram, R., *Circular Economy*, 2**024**, *3*, 10007
2. Boneta, S.; Arafet, K.; Moline, V., *J. Chem. Inf. Model.*, **2021**, *6*, 3041.
3. Hong, H.; Ki, D.; Seo, H.; Park, J.; Jang, J.; Kim, K. –J., *Nat. Commun.*, **2023**, *14*, 4556.

OP 18

Green-Synthesized Biomass-Derived Carbon Dots for Sensitive and Selective Detection of Pesticide

Arya P.B.[a], Renuka N. K.[a,*]

[a]*Materials Engineering Lab, Department of Chemistry, University of Calicut, India*

[*]*renuka@uoc.ac.in*

Keywords: Cypermethrin, Fluorometric sensing, Fruit peel, Biomass-derived Carbon dots

Ensuring food safety is vital to human health, as contamination by toxic chemicals poses serious health threats. In this direction, pesticide contamination in food is one of the grieve issue to be addressed. Cypermethrin, a widely used synthetic pyrethroid insecticide, though effective in pest control, can penetrate the blood–brain barrier and cause neurotoxic effects, convulsions, and even fatality upon prolonged exposure[12]. Hence, developing a rapid, sensitive, and eco-friendly detection method for cypermethrin is of great importance. In this study, environmentally benign carbon dots (CDs) are synthesized from pomegranate peel via a simple hydrothermal method and employed as a fluorescent probe for cypermethrin detection. The synthesized pomegranate peel-derived carbon dots (PPCDs) exhibit strong blue fluorescence under UV excitation. Upon interaction with cypermethrin, the fluorescence intensity of PPCDs was effectively quenched due to a static quenching mechanism, enabling quantitative detection. The fluorescence quenching displayed strong linearity with an R^2 value of 0.99196 and a limit of detection (LOD) of 3.703 μM. The study presents the first standalone application of green-synthesized carbon dots for highly selective, sensitive, and cost-effective fluorescence detection of cypermethrin, demonstrating excellent selectivity against 32 potential interfering analytes and highlighting their potential as sustainable nanosensors for monitoring pesticide residues in food and environmental samples.

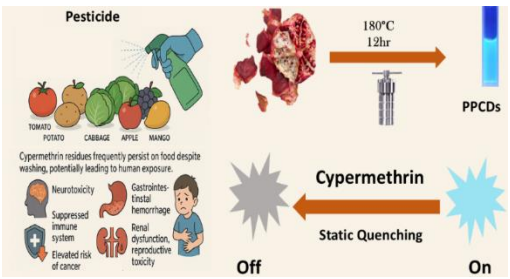


Figure 1 Schematic Representation Highlighting the Health Risks Associated with Cypermethrin Exposure and Its Sensitive Detection Using Eco-Friendly Pomegranate Peel-Derived Carbon Dots (PPCDs)

References

1. Kaur, R.; Singh, J., *Nat. Environ. Pollut. Technol.*, **2021**, *20*, 1997–2005.
2. Muhammad, M.; Khan, S.; Rahim, G.; Alharbi, W.; Alharbi, K. H., *Environ. Monit. Assess.*, **2022**, *194*, 890.

OP 19

Direct Synthesis of Amides from Nitro Compounds and Alcohols *via* Borrowing Hydrogenation

Padmavathy V. K. Nair[a], Gourishankar B. Swami[a] and Boopathy Gnanaprakasam[a,*]

[a]*Department of Chemistry, Indian Institute of Science Education and Research, Pune, India*

[*]*gnanaprakasam@iiserpune.ac.in*

Keywords: Borrowing hydrogenation, Alcohol dehydrogenation, Ruthenium catalyst, Amidation, Nitro compound reduction.

Despite tremendous advancements in the synthesis of amides using various organic transformations, the efforts to eliminate waste associated with these protocols have failed to meet with success.[1] Generally, amines required for the amidation reaction are obtained from their respective nitro compounds[2] which increases the steps in the reaction and generates associated waste. Consequently, an environmentally benign, sustainable and efficient means of accessing amides is in high demand. Hence, direct amidation from nitro compounds by a catalyst without isolating the intermediates using borrowing hydrogenation strategy is greener, more efficient and sustainable in contemporary chemical synthesis.[3,4]

Herein, we have discovered a direct amidation reaction using readily available nitro compounds and alcohols via a catalytic borrowing hydrogen method with water as the by-product (Fig. 1).[5] This reaction is catalyzed by 10 mol% of Ru-catalyst and goes through multiple reactions, including oxidation of alcohol, reduction of nitro group and formation of amides in a tandem sequence in one pot condition. This reaction provides a step economic advantage over the available techniques, tolerates various functionalities, and has been demonstrated with a broad scope (47 examples) of amides.

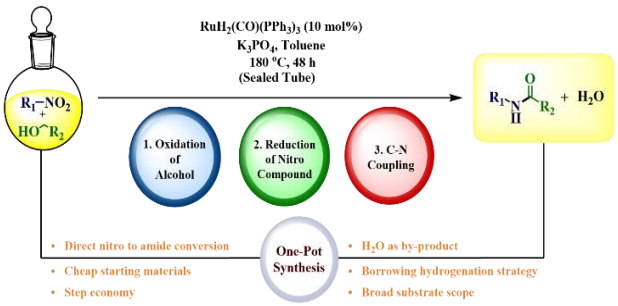


Figure 1: Ruthenium Catalyzed Direct Amidation of Nitro compounds with Alcohol via Borrowing Hydrogenation[5]

References

1. Pattabiraman, V. R.; Bode, J. W., *Nature* **2011**, *480*, 471– 479.
2. Tafesh, A. M.; Weiguny, J., *Chem. Rev.* **1996**, *96*, 2035-2052.
3. Xiao, F.; Liu, Y.; Tang, C.; Deng, G. J., *Org. Lett.* **2012**, *14*, 984-987.
4. Xiong, N.; Dong, Y.; Xu, B.; Li, Y.; Zeng, R., *Org. Lett.* **2022**, *24*, 4766-4771.
5. Nair, P. V. K.; Swami, G. B.; Gnanaprakasam, B., *Org. Lett*. **2025**, *27*, 3560-356 .

OP 20

Convergent Synthesis of Coumarin C3–C4-Fused Fluorogenic Quinoline Scaffolds *via* Aldehyde Activation using in situ Generated Hydrazoic Acid

Ranjithkumar Ganesan[a], Sriraghavan Kamaraj[a,*]

[a]*Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India.*

*****sriraghavan.k@vit.ac.in*

Keywords: Azido-coumarin, Fluorogenic quinoline, In situ hydrazoic acid, Pomeranz–Fritsch-type cyclization

The article describes an efficient route for the construction of diversely substituted coumarin C3-C4 fused quinoline from pre-functionalized 4-azido-3-formylcoumarin using various aromatic/heterocyclic amines in excellent yield with a focus on application-oriented substrates scope. This protocol provides a straightforward synthesis of fluorogenic coumarin-fused quinoline scaffolds through aldehyde activation by 'in-situ' generated HN_3 with excellent atom economy. Our synthetic methodology has been showcased and applied by synthesizing 31 structurally diversified scaffolds, the gram-scale experiment, and structural validation with four single-crystal XRD studies. Also, we have proposed a plausible mechanistic pathway from the control experimental studies. Fascinatingly, the remarkable features of this methodology include, without the intervention of secondary products, excellent yield, chromatography-free isolation, functional group compatibility, and tolerance of electron influence of different substituents, which makes this methodology ideal for the construction of CQ scaffolds.

References

1. Marshall, C. M.; Federice, J. G.; Bell, C. N.; Cox, P. B.; Njardarson, J. T., *J. Med. Chem*. **2024**, *67*, 11622–11655.
2. Thigulla, Y.; Kumar, T. U.; Trivedi, P.; Ghosh, B., *ChemistrySelect* **2017**, *7*, 2718–2721.
3. Patra, P.,*ChemistrySelect* **2019**, *4*, 2024–2043.
4. Kumari, S.; Shakoor, S. M. A.; Markad, D.; Mandal, S, K., *Eur. J. Org. Chem*. **2019**, 705–714.
5. Lu, Z.; Zhang, Q.; Chen, R.; and Yu, D., *J. Asian Nat. Prod. Res*. **2008**, *10*, 37–41.

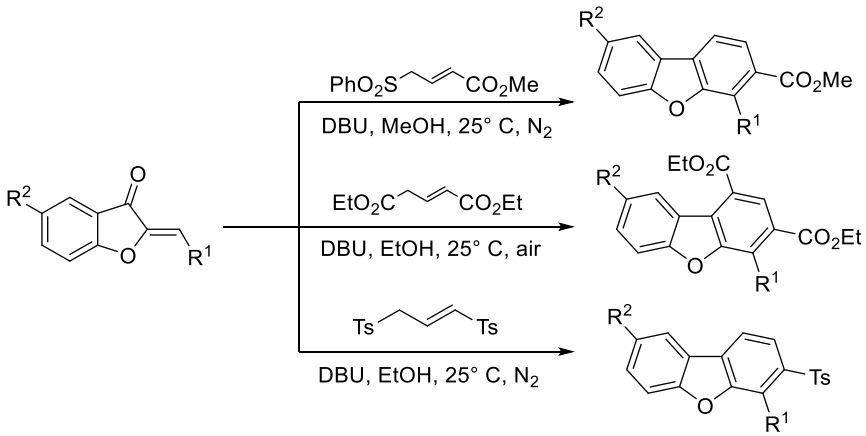
OP 21

Synthesis of Dibenzofuran Derivatives *via* Base-mediated [3+3] Benzannulation Reactions

Farooqe Husni P.[a], Rajeev S. Menon [a,*]
[a]*Department of Chemistry, University of Calicut, Kerala 673 635*
[*]*rajeev@uoc.ac.in*

Keywords: Benzannulation, Dibenzofuran

A facile DBU-mediated [3+3] benzannulation reactions[1] of aurone derivatives with three different 1,3-bis nucleophiles to yield substituted dibenzofurans is described. Aromatization occurs via either aerial oxidation or elimination pathway. The following two-fold selectivity is a stand-out feature of the method: (i) sulfonyl bearing substrates react selectively via the elimination pathway, and (ii) they react with exclusive regioselectivity.[2] The method has a broad substrate scope and dibenzofurans decorated with substituents at well-defined positions are formed. The reaction can also be carried out as a one-pot, three-component operation using benzofuranone, the corresponding aldehyde, and 1,3-bis nucleophile. The products could be easily transformed into dibenzofurano-coumarins, a scaffold known to show cytotoxic activity.[3]



Scheme 1: [3+3] Benzannulation of Aurone with different 1,3-bisnucleophiles

References

1. Swami, B.; Yadav, D.; Menon, R. S., *Chem. Rec.* **2022**, *22*, e202100249.
2. Joshi, P. R.; Undeela, S.; Reddy, D. D.; Singarapu, K. K.; Menon, R. S., *Org. Lett.* **2015**, *17*, 1449–1452.
3. Oliveira, A. M. A. G.; Raposo, M. M. M.; Oliveira-Campos, A. M. F.; Machado, A. E. H.; Puapairoj, P.; Pedro, M.; Nascimento, M. S. J.; Portela, C.; Afonso, C.; Pinto, M., *Eur. J. Med. Chem.* **2006**, *41*, 367–372.

POSTER PRESENTATIONS

PP 01

Designing Chelates for Detection and Detoxification of Toxic Metal Ions in Animal Tissues

Cyril Augustine [a, b*], Tiju Thomas [b]

[a] *Department of Chemistry, St. Berchmans College (Autonomous), Kottayam, India.*
[b] *Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India*
**cyril@sbcollege.ac.in*

Keywords: Toxic Metals, Detoxification, Mercury

Mercury compounds, both organic and inorganic, pose serious hazards when released into the environment. Existing techniques for the simultaneous detection and detoxification of Hg(II) in biological and environmental samples remain inadequate. A promising approach involves a selective fluorescent sensor, derived from Pyronin Y (Py) and meso-2,3-dimercaptosuccinic acid (DMSA). This study explores the chemistry of the sensor through Density Functional Theory (PBE1PBE/def2tzvp), focusing on its interactions with Hg (II). Computational analysis of thermochemical parameters reveals the spontaneity of dissociation and complex formation, as indicated by Gibbs free energy changes ($\Delta_r G°$). The combined experimental and theoretical insights highlight the potential of such sensors for detecting and detoxifying toxic metals.

References

1. Rivera-Méndez, M. A.; Navarro, E.; Martínez-Rodríguez, E.; Hernández, C.; López. R.; Rubio. M, *Coord. Chem. Rev*., **2020**, *425*, 213498.
2. Flora. G.; Gupta. D.; Tiwari. A., *J. Trace Elem. Med. Biol*., **2019**, *54*, 226–231.
3. Kosnett. M. J., *J. Toxicol*., **2010**, *2010*, 1–12.

PP 02

Removal of Hardness from Wastewater Using an Ion Exchange Resin

Kalyani M. Naik[a], Nupur M. Jalewar[a], Anusaya S. Chavan[a,*]
[a]*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Maharashtra, India*
[*]*aschavan.chemistry@bamu.ac.in*

Keywords: Ion exchange resin, Hardness of water, Ion exchange capacity, Waste water treatment, Parameters.

Water hardness, primarily caused by the presence of calcium (Ca^{2+}) and magnesium (Mg^{2+}) ions, poses challenges in domestic, industrial, and environmental applications by leading to scaling, reduced soap efficiency, and equipment damage. Ion exchange resins offer an efficient and widely adopted method for hardness removal. In this study, a cation exchange resin was employed to replace divalent hardness-causing ions with sodium ions, thereby softening the water.

The efficiency of the process was evaluated by monitoring the hardness of wastewater before and after treatment using a standard analytical technique.[1-3] Batch experiments were conducted to evaluate the influence of different parameters on ion exchange resin capacity, such as flow rate, column size, and temperature.[4] Results demonstrated a significant reduction in hardness, confirming the applicability of ion exchange resins as a cost-effective and sustainable method for wastewater treatment. Other details will be debated during the presentation.

References

1. Joshi, A.; Hande, S.; Chorghade, V.; Devale, P.; Gargade, P., *J.Natl. Res. Dev.,* **2023,** *8*, 26-28.
2. Ali, A.; Sadia, M.; Azeem, M.; Ahmad, M.; Umar, M.; Abbas, Z., *Futur. Biotechnol.,* **2023,** *3*, 12-19.
3. Jahagirdar, D. V., *Experiments in Chemistry*, **1994** (1st ed).
4. Jeffery, G.; Bassett, J.; Mendham, J.; Denney, R., *Vogel's textbook of quantitative inorganic analysis.,***1989**.

PP 03

Adsorptive Behavior of $ZnFe_2O_4$ Nanoparticles with Bi^{3+} Doping for the Removal of Cr (VI) from Aqueous Solution

Mariyam Thomas[a,*], Aruna Joseph[b], Thanooja Nizam[c]

[a]*Department of Physics, St. Teresa's College, Ernakulam, Kerala, India*

[b]*Centre for Advanced Functional Materials, Department of Physics, Bishop Moore College, Alappuzha, Kerala, India*

[c]*Department of Physics, Mar Ivanios College, Thiruvananthapuram, Kerala, India*

[*]*mariyamthomas@teresas.ac.in*

Keywords: Ferrite, Adsorption, Heavy metal removal

Water is essential for the survival of all living organisms and the proper functioning of ecosystems. However, only about 0.014% of the total water on Earth is freshwater suitable for consumption, and humans utilize approximately 36% of this limited resource.[1] Increasing pollution from heavy metals, pathogens, dyes, surfactants, and radioactive substances has made much of the available water unsafe for use. Heavy metals, in particular, enter the environment through natural processes and human activities such as electroplating, battery recycling, metal smelting, and industrial emissions. Among these, hexavalent chromium [Cr (VI)] is of major concern due to its high mobility, solubility, and toxicity.[2] Therefore, its effective removal from wastewater is critical. Several techniques such as adsorption, ion exchange, electrochemical treatment, membrane filtration, and reverse osmosis have been explored for this purpose. In the present study, adsorption using $ZnFe_2O_4$-based nanoparticles has been employed as an efficient and economical method for Cr (VI) removal.

The present study investigates the effectiveness of sol–gel-derived $ZnFe_{2-x}Bi_xO_4$ (x = 0.0, 0.05, 0.10, 0.15, 0.20) nanoparticles for the removal of Cr (VI) ions from aqueous solutions. Batch adsorption experiments were conducted to evaluate the influence of various parameters, including contact time, adsorbent dosage, pH, initial ion concentration, and temperature. The adsorption process was found to follow a monolayer adsorption mechanism consistent with the Langmuir isotherm model and pseudo-second-order kinetics.[3,4] Among the synthesized samples, $ZnFe_{1.9}Bi_{0.1}O_4$ exhibited a markedly higher adsorption efficiency compared to $ZnFe_2O_4$, demonstrating its potential as an effective and economical material for heavy metal removal from wastewater. Quantitative analyses of adsorption were performed using Atomic Absorption Spectroscopy (AAS), and the results revealed that Bi^{3+} doping significantly enhanced the adsorption capacity, attributed to the increased effective surface area and improved electrostatic charge density on the nanoparticle surface.

References

1. Bharti, M.K.; Gupta, S.; Chalia, S.; Garg, I.; Thakur, P.; Thakur, A., *J. Supercond. Nov. Magn.*, **2020,** *33*, 3651-3665.
2. Duruibe, J. O.; Ogwuegbu, M. O. C.; Egwurugwu, J. N., *Int. J.Phys.Sci.*, (**2007**), 2, 112-118.
3. Song, S.; Peng,W.; Li, H, *Chem. Mat. Sci.*, **2020**, Springer.

PP 04

Metal Complexes of Pillar [5] arene Derivative for the Selective Detection of Amino Acids and Anions in Water

Marzoq. A. Aldharhani[a, b], Roymon Joseph[a,*]

[a] *Department of Chemistry, University of Calicut, Thenjhipalam, Kerala, India - 673635.*

[b]*Department of Chemistry, Applied and Human Science College, Amran University, Amran, Yemen – 009677.*

[*] *roy@uoc.ac.in*

Keywords: Pillar[5]arene, Metal ions, Anions, Amino acids, Host-guest interactions.

The detection of ions and molecules is an intriguing area of research owing to its importance in biology and environment. The macrocycles functionalized with appropriate binding groups are known for the selective detection of various analytes. In this study, we synthesized a water-soluble, Sulphur-functionalized pillar[5]arene containing ten carboxylic acids groups (**TPA**) and characterized it using ^{1}H and ^{13}C NMR spectroscopy along with high-resolution mass spectrometry. The **TPA** was found to form complexes with Fe^{3+}, Cu^{2+}, and Hg^{2+}, as evidenced by variations in its absorbance and fluorescence intensity. The metal-**TPA** complexes exhibited versatility as optical probes, demonstrating secondary sensing abilities toward different amino acids and anions. The *in-situ* prepared Fe^{3+} complex of **TPA** (**FeTPA**) displayed selective detection of L-tyrosine among the naturally occurring amino acids, with a limit of detection of 488 ± 44 nM. In contrast, the Cu^{2+} and Hg^{2+} complexes of **TPA** (**CuTPA** and **HgTPA**) exhibited selectivity towards L-cysteine, with a detection limit of 610 ± 3 nM and 1.29 ± 0.23 µM, respectively. Interestingly, the Cu^{2+} complex of **TPA** (**CuTPA**) is found to be selective for S^{2-} ion among 14 anions with a detection limit of 326 ± 18 nM. All the interaction between the metal complexes and the amino acids or anions were studied by UV-visible and fluorescence spectroscopy. The detection of amino acids by the **TPA**-metal complexes operates through a displacement mechanism, in which the incoming amino acids displaces the metal ion from the **TPA** binding core resulting in the formation of free **TPA** and amino acid-metal complexes in solution. The present study highlights the versatility of supramolecular–metal complexes in the selective recognition of analytes and serves as a model for the rational development of multifunctional sensing materials.

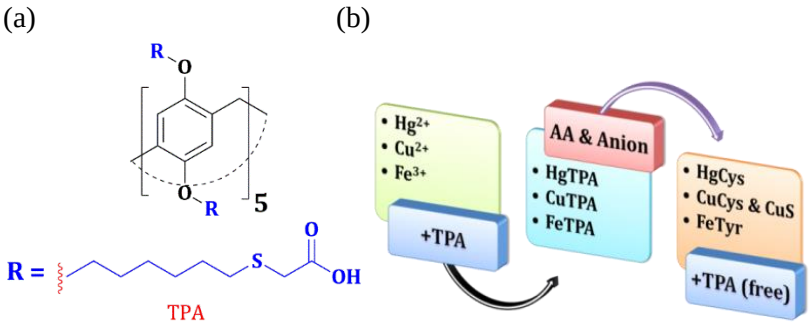


Figure 1(a): Structure of TPA (b): Sensing diagram of Amino acid and Anions

References

1. Ogoshi, T.; Yamagishi, T. A.; Nakamoto. Y., *Chem. Rev*., **2016**, *116*, 7937-8002.
2. Joseph, R. *ChemistrySelect*, **2021**, *6*, 3519-3533.
3. Chen, J. F.; Liu, X.; Ma, J. F.; Han B. B.; Ding, J. D.; Lin. Q.; Yao. H.; Zhang, Y. M.; Wei. T. B, *Soft matter*, **2017,** *13*, 5214-5218.

PP 05

A Sustainable Method for the Complete Removal of Heavy Metals from Polluted Water Using Phyotogenic Cubic Ceria Nanoparticles

Sreelakshmi T[a], Dr. Abraham Joseph[a,*]

[a]*Department of Chemistry, University of Calicut, Calicut University, Kerala, India.*

**abrahamjoseph@uoc.ac.in*

Keywords: Phytogenic ceria; Physicochemical methods; Mesoporous materials; Adsorption isotherm.

Cerium oxide nanoparticles were synthesized via an eco-friendly green approach using plant extract and assessed for their potential as adsorbents in removing heavy metals from contaminated water. Comprehensive structural and surface characterization through XRD, FTIR, SEM–EDX, TEM, BET, and XPS confirmed the formation of mesoporous cubic CeO_2 with an average crystallite size of approximately 21.6 nm. The nanoparticles demonstrated exceptional adsorption efficiency, exhibiting maximum adsorption capacities (Q_m) of 730.1 mg g^{-1} for Pb(II). The adsorption process conformed to the Langmuir isotherm, indicating monolayer adsorption, while the kinetics followed a pseudo-second-order model. Almost complete removal was achieved, with 100% elimination of Pb(II) ions. Furthermore, the influence of solution pH and coexisting ions was systematically investigated, confirming the adsorbent's robustness and selectivity under diverse water conditions. Overall, the study emphasizes the superior efficiency and sustainability of green-synthesized CeO_2 nanoparticles as a promising material for heavy metal remediation[1-3].

References

1. Olivera, S.; Chaitra, K.; Venkatesh, K.; Muralidhara, H. B.; A. M., Ahamed, M. I., *Environ. Chem. Lett.*,**2018,** *16*, 1233-1246.
2. Sirimongkol, M. M.; Ayawanna, W. J., *Mater. Chem. Phys.*, **2018,** *214*, 56-65.
3. Biswas, A.; Chandra, B., *Appl. Surf. Sci.*, **2023,** *612*, 155841.

PP 06

Design and Synthesis of Thiadiazole-Based Compounds

Akash R. Pawar[a], Nupur M. Jalewar[a], Anusaya S. Chavan[a,*]

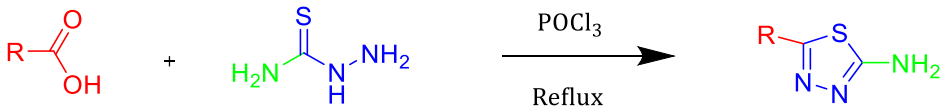
[a]*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Maharashtra, India*

**aschavan.chemistry@bamu.ac.in*

Keywords: Thiadiazole, Thiosemicarbazide, Phosphorus oxychloride, Cyclisation, Biological activity.

Thiadiazole derivatives represent an important class of heterocyclic compounds known for their diverse biological and pharmaceutical activities, including antimicrobial, anti-inflammatory, and anticancer properties.[1-3] In the present study, a series of thiadiazole-based compounds was synthesised by the cyclisation of various carboxylic acids with thiosemicarbazide in the presence of phosphorus oxychloride ($POCl_3$) as a dehydrating and cyclizing agent (Scheme 1).[4] The reaction proceeded efficiently, yielding the desired thiadiazole derivatives in good yields under mild conditions. The synthesised compounds are planned to be characterised by spectroscopic techniques to confirm their structures. This convenient synthetic approach offers a promising route for developing biologically active thiadiazole scaffolds for future pharmacological studies. Other details will be debated during the presentation.

Scheme 1:



1 **2** **3**

References

1. Górecki, S.; Kudelko, A.; Olesiejuk, M., *Pharmaceuticals*, **2025**, *18*, 1348.
2. Kadam, S.; Kabra, R.; Ganure, A., *Int. J. Curr. Pharm. Sci.*, **2015**, *1*, 207-215.
3. Santhosh, C. R.; Chinnam, S.; Kottam, N.; Amreen, S.; Ananthnag, G. S.; Madhu, G. M.; Gadde, S.; Fernandes, V. T.; Arnipalli, H., *Results Chem.*, **2025**, *13*, 101939.
4. Ramprasad, J.; Nayak, N.; Dalimba, U., *Eur. J. Med. Chem.*, **2015**, *106*, 75-84.

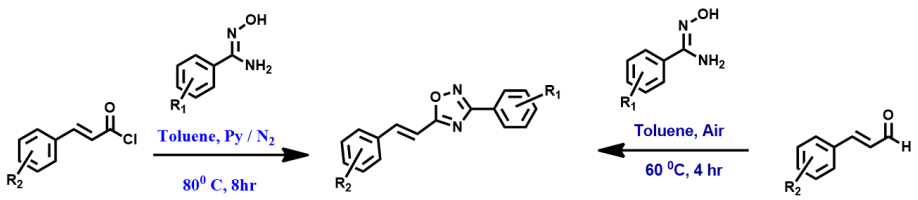
PP 07

Facile Synthesis of Novel Styryl 1,2,4-Oxadiazole Derivatives from Amidoximes

Arathi T. Parambu [a], Gopika K [a], Amritha A [a], Suja T D[a,*]
[a]*Department of Chemistry, University of Calicut, India, 673635*
**suja@uoc.ac.in*

Keywords: Oxadiazole, Amidoxime, Heterocycle

1,2,4-Oxadiazole is a highly versatile heterocyclic scaffold that finds extensive applications in areas such as agrochemicals, materials science, and drug development, owing to its remarkable structural and functional properties.[1,2] Amidoximes, which are easily accessible from nitriles, has been shown to be a highly useful building block for the construction of this valuable heterocyclic system.[3] We have developed a convenient, one-step synthesis of styryl oxadiazoles from amidoximes and cinnamaldehyde or cinnamoyl chloride derivatives. This thermal and base-promoted condensation-cyclization cascade installs the 1,2,4-oxadiazole framework with remarkable efficiency. A series of structurally diverse disubstituted 1,2,4-oxadiazole derivatives were readily synthesized. The developed method is a simple, efficient, economical and green protocol utilizing easily available, non-toxic substrates and solvents, without any catalysts or oxidants.



Scheme 1. Synthesis of styryl1,2,4-oxadiazole

References

1. Pace, A.; Pierro, P.. *Org. Biomol. Chem.*, **2009**, *7*, p. 4337-4348.
2. Upare, A.A., et al., *Bioorg. Chem.*, **2019**, 86, 507-512.
3. Baykov, S., et al., *Tetrahedron Lett.*, **2020**, *61*,152403.

PP 08

Visible-Light Enabled Organophotoredox Catalysis: A Sustainable Approach to Sulfonylation Reactions

Archana Vijayakumar[a], Manod M[a], Chithra Mohan[a,*]

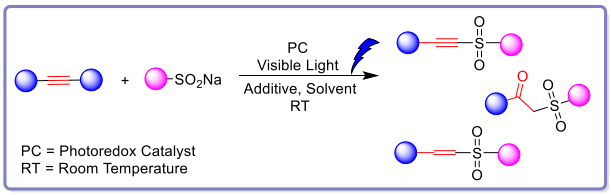
[a]*School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala, India-686560*

**chithramohan84@mgu.ac.in*

Keywords: Organophotoredox catalysis, Visible light, Alkynes, Sulfonylation, Metal-free

Organosulfur compounds have garnered immense interest among synthetic organic chemists owing to their significance in medicinally and pharmaceutically active molecules.[1] Photoredox catalysis utilizes visible light employing catalysts to initiate redox reactions via single-electron transfer, producing milder and more sustainable transformations.[2,3] Visible-light-mediated synthesis of sulfones, sulfides, and several other sulfur-containing heterocycles has been reported extensively in the past few decades, since they do not involve harsh reaction conditions, restrictive substrate scope, expensive and toxic metals and ligands, and over-stoichiometric amounts of oxidants, the common challenges of conventional synthetic routes.[4,5]

In this work, we explore a novel synthetic protocol for the construction of C-S bonds through visible light-enabled organophotoredox catalysis under transition metal-free conditions (Scheme 1). Various alkynes, sulfinic acid, and a photocatalyst are irradiated with visible light of a suitable wavelength. Visible-light-enabled photoredox catalysis is an efficient and facile strategy to achieve C-S bond construction.



Scheme 1. Visible-light enabled sulfonylation and oxysulfonylation of alkynyl derivatives.

References

1. Zhu, J.; Yang, W. C.; Wang, X. D.; Wu, L., *Adv. Synth. Catal.* **2018**, *360*, 386–400.
2. Shaw, M. H.; Twilton, J.; MacMillan, D. W. C., *J. Org. Chem.* **2016**, *81*, 6898–6926.
3. Romero, N. A.; Nicewicz, D. A., *Chem. Rev.* **2016**, *116*, 10075–10166.
4. Wu, H.; Chen, S.; Liu, C.; Zhao, Q.; Wang, Z.; Jin, Q.; Sun, S.; Guo, J.; He, X.; Walsh, P. J.; Shang, Y., *Angew. Chemie., Int. Ed.* **2024**, *63*, 1–9.
5. Jin, Z.; Yu, T.; Wang, H.; Jia, P.; Huang, Y., *Org. Chem. Front.* **2024**, *11*, 6573–6588.

PP 09

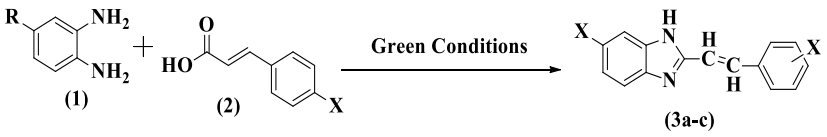
Synthesis, *In-vitro* antimycobacterial evaluation and docking studies of some new 2-heterostyrylbenzimidazole compounds as Inhibitors of *Mycobacterium tuberculosis* Pantothenate Synthetase

Ashok Kumar Taduri[a,*], Rama Devi Bhoomireddy[b],
[a]*Department of Chemistry, JNTUH University College of Engineering, Science & Technology Hyderabad, Telangana, India – 500085.*
[*]*ashok.jntu@gmail.com*

Keywords: 2-heterostyrylbenzimidazoles, Mycobacterium tuberculosis.

Tuberculosis is one of the oldest documented infectious disease and threat to worldwide public health, mainly caused by *Mycobacterium tuberculosis (M.tb.)* bacteria species. It is the only disease that does not require any vector for transformation from one person to another.[1] In 2010, there were around 8.8 million incident cases of TB, and around 1.1 million deaths from TB among HIV-negative people, and an additional 0.35 million deaths from HIV-associated TB.[2]

Cinnamic acids, its derivatives such as ethyl cinnamate, sodium cinnamate, and benzylcinnamate have century old history as potential antituberculosis agents. 2-Styrylbenzimidazoles which were synthesized from these Cinnamic acids are also showed promising antituberculosis activity, but the practicable greener routes available for the synthesis of novel 2-heterostyrylbenzimidazoles are very less in the literature. Herein, we report the facile synthesis of some novel 2-heterostyrylbenzimidazoles using greener routes which were tested against *Mycobacterium Tuberculosis* and other Gram positive and Gram negative bacteria.



R = H, NO_2 ,-COPh
X = H, CH_3, Cl, F, NO_2

Pantothenate synthetase (PS) was considered as the target for the molecular docking studies and evaluated the binding pattern at active site, as PS plays a significant role in the biosynthesis of pantothenate in *Mycobacterium tuberculosis* (MTB).

References

1. Dutt, A. K.; Stead, W. W., *Epidemology and Host Factors: Tuberculosis and Nontuberculosis Mycobacterial Infection*, W. B. Saunders Company, Philadelphia, Pa, USA, 4th Edition, **1999**.
2. World Health Organization Report 2011: Global Tuberculosis Control,WHO/HTM/TB/2011.16.

PP 10

Design and Synthesis of Substituted Quinoline–Chalcone Derivatives as Nitrogen-Based Heterocyclic Scaffolds

Ashvini A. Jadhav[a], Anusaya S. Chavan[a,*]

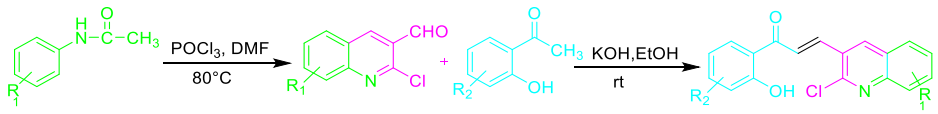
[a]*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Maharashtra, India*

**aschavan.chemistry@bamu.ac*

Keywords: Medicinal sciences, Chloroquinoline

Nitrogen-containing heterocycles form the backbone of many biologically active molecules and functional materials. In this study, a novel chloroquinoline-chalcone derivatives was designed, synthesized, and characterized. The synthesis was achieved through a straightforward and efficient route, affording good yields under mild conditions. The findings highlight the significance of chloroquinoline–chalcone derivatives as versatile scaffolds with potential applications in pharmaceutical and medicinal sciences. The said details and other aspects will be debited.

Scheme:-



References

1. Liu, M.; Wilairat, P.; Croft, S. L.; Tan, A.L.; M. Go, M., *Bioorg. & Med. Chem.* **2003**, *11*, 2729–2738.
2. Mokle, S. S.; Vibhute, Y. B., *Der Pharma Chemica*. **2009**, *1*, 145-152.
3. Radhakrishnan, S. K.; Shimmon, R. B.; Conn, C.; Baker, A. T., *Bioorg. & Med. Chem. Lett.* **2015**, *25*, 1753–1756.
4. Kumara, D.; Kaushikb, M., *Russ. J. Org. Chem.* **2023**, *59*, 1059–1063.

PP 11

Analysis of Non- Alcoholic Beverages

Attadip K. Bhadarge[a], Nupur M. Jalewar[a], Anusaya S. Chavan[a,*]
[a]*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Maharashtra, India*
**aschavan.chemistry@bamu.ac.in*

Keywords: Non-alcoholic beverages, Nutritional contribution, Caffeine, Soft drinks, Energy drinks.

Non-alcoholic beverages constitute a rapidly growing segment of the food and beverage industry, valued for their wide consumer acceptance and nutritional contribution.[1] This study focuses on the analysis of selected non-alcoholic beverages, including soft drinks and energy drinks, to evaluate their caffeine content and quality parameters. This study emphasizes the importance of analytical quality assessment for ensuring consumer safety, product labelling accuracy, and regulatory compliance in the non-alcoholic beverage sector.[2,3] Other details will be debated during the presentation.

References

1. Rana, P.; Mishra, M., *Int. J. Forensic Sci.*, **2023**, *6*, 97-103.
2. Ogbeide, U.; Irene, D.; Okeri, H., *J. Sci. Pract. Pharm.*, **2021**, *8*, 441-446.
3. Asogwa, F.; Ugodi, G.; Ebugosi, R.; Achara, I.; Achieti-Atim, H., *Glob. J. Pure Appl. Sci*., **2023**, *29*, 1-10.

PP 12

Comparison of Nutrient Value of Different Types of Eggs (Rural and Broiler)

Avinash P. Gawai[a], Nupur M. Jalewar[a], Anusaya S. Chavan[a,*]
[a]*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Maharashtra, India*
**aschavan.chemistry@bamu.ac.in*

Keywords: Country eggs, Broiler eggs, Nutritional value, Micronutrients, Antioxidants.

Eggs are recognized as an affordable and highly nutritious food, supplying essential proteins, fats, vitamins, and minerals to human diets.[1] Among the commonly consumed varieties, country eggs and broiler eggs show notable differences in nutritional value, availability, and market price. Country eggs, which are generally more than four times costlier than broiler eggs, are considered more natural, with lower fat content and higher levels of micronutrients and antioxidants. These qualities make them valuable for improving immunity and supporting overall health.

In contrast, broiler eggs are larger in size, contain higher amounts of protein and fat, and are more affordable and widely available, making them a practical choice for meeting daily nutritional requirements. This study aims to compare the usability, benefits, and consumer preferences of country eggs and broiler eggs, highlighting their respective roles in nutrition and health.[2,3] Other details will be debated during the presentation.

References

1. Caffa, I.; Proietti, E.; Turrini, F.; Borgarelli, C.; Ferrando, M.; Formisano, E.; de Cassya Lopes Neri, L.; Martini, D.; Angelino, D.; Tagliabue, A.; Pisciotta, L., *Food Sci. Nutr*., **2025**, *13*, 70285.
2. Jahagirdar, D. V., *Experiments in Chemistry*, **1994** (1st ed), Himalaya Publishing House, Bombay, India.
3. Amir, R.; Iftikhar, H.; Amjad, A., *GSJ*, **2021**, *9*, 1134-1136.

PP 13

Tröger's Base-Based Fluorescent Organic Polymers for Selective Detection of Phenylglyoxylic Acid in Urine: A Biomarker of Styrene Exposure

Harsha Gangadharan[a], Sumithra L[a], Sankarasekaran Shanmugaraju[a,*]
[a]*Department of Chemistry, Indian Institute of Technology Palakkad, Palakkad-678623, Kerala, India*
**202414009@smail.iitpkd.ac.in*

Keywords: Organic polymers, Tröger's Base, Fluorescent sensing, Phenylglyoxylic acid

Styrene, a major raw material in plastic and synthetic rubber production, is known to emit volatile compounds into the environment. Once absorbed by the human body, styrene is metabolized into phenylglyoxylic acid (PGA), which is then excreted in urine. The International Agency for Research on Cancer (IARC) classifies PGA as a Group 2B substance, indicating its potential to cause cancer. Therefore, accurately and selectively detecting PGA in biological fluids is highly important for both analysis and biomedical purposes. In this study, we report the synthesis of a fluorescent porous organic polymer that incorporates Tröger's base (TB) units for detecting PGA in urine samples. Tröger's base - a rigid, V-shaped, nitrogen-bridged bicyclic compound - has a unique three-dimensional molecular structure with inherent chirality and electron-rich nitrogen sites. These features make TB an excellent scaffold for creating porous organic frameworks with adjustable fluorescence and selective binding abilities. The synthesized TB-based polymer was thoroughly characterized and tested as a fluorescence sensor. When interacting with PGA, the polymer showed significant fluorescence quenching, enabling sensitive and selective detection even amid other competing analytes. This group of PGAs and the electron-rich TB framework, likely involving hydrogen bonding and π–π stacking interactions. The polymer demonstrated excellent stability, porosity, and reproducibility, highlighting its potential as a durable material for bioanalytical sensing. Ongoing studies aim to evaluate its use in real-time detection systems for practical applications.

References

1. Song, D; Ji, X; Li, Y; Wu, S; Zhang, Y; Wang, X; Sun, Y; Gao, E; Zhu, M, *Dalton Trans*., **2022**, *51*, 16266.
2. Tong, R; Luo, R; Wang, W; Lu, H; Li, Y; Zhang, D; Wang, Y; Li, Z; Shao, F, *Cryst. Growth Des.*, **2024**, *24*, 7212-7221.
3. Jia, P; Gao, L; Zheng, Y; Wang, C; Yang, C; Li, Y; Zhao, Y, *ACS Appl. Mater. Interfaces*, **2021**, *13*, 33546-33556.

4. Ji, C; Zhang, J; Fan, R; Sun, T and Yang, Y, *ACS Appl. Mater. Interfaces*, **2023**, *15*, 51796-51805
5. Hui, Z; Luo, R; Gang, R; Li, Y; Zhang, D; Chen, D; Wu, X; Shao, F, *Cryst. Growth Des.,* **2025**, *25*, 508−518.

PP 14

Designing Cyclic Peptide Binders for Inhibition of HLA-DP2 – TCR Targeting Protein-Protein Interaction

Aneena Hakkim Kattumunda[a], Radhika Narayanan Nair[b], Anjali Nishad Minimol[b], Susmita De[b,*]

[a]*Department of Zoology, University of Calicut, Malappuram – 673635, Kerala, India*
[b]*Department of Chemistry, University of Calicut, Malappuram – 673635, Kerala, India*
**susmita@uoc.ac.in*

Keywords: Cyclic peptides, Hypersensitivity, HLA

Chronic beryllium disease (CBD) is a granulomatous lung disease resulting from beryllium hypersensitivity. The condition is characterized by accumulation of $CD4^+$ T-cells specific to beryllium in the lungs.[1] The interaction of T-cell receptors (TCRs) with Be^{2+} bound class II Major Histocompatibility Complex (MHC) molecules, specifically HLA-DP2 plays a key role in initiating the progression of the disease.[2] By employing computational modelling techniques, particularly the cPEPmatch method, and evaluations using molecular dynamics simulations, cyclic peptides with potential to inhibit the protein-protein interaction between HLA-DP2 and TCR can be designed, thereby offering potential therapeutic strategies for controlling aberrant immune responses associated with CBD.[3] Combinations of cyclic peptide candidates were used to attain higher binding energy for effective modulation [Figure 1].

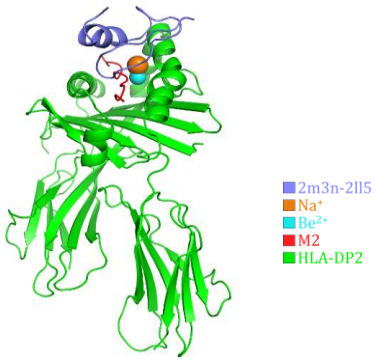


Figure 1: HLA-DP2_M2_Be^{2+} shown complexed with cyclic peptide combination 2m3n-2ll5.

References

1. Clayton, G. M.; Wang, Y.; Crawford, F.; Novikov, A.; Wimberly, B. T.; Kieft, J. S.; Falta, M. T.; Bowerman, N. A.; Marrack, P.; Fontenot, A. P.; Dai, S.; Kappler, J. W., *Cell*, **2014**, *158 (1)*, 132–142.
2. Fontenot, A. P.; Kotzin, B. L.; Comment, C. E.; Newman, L. S., *Am J Respir Cell Mol Biol*, **1998**, *18 (4)*, 581–589.
3. Santini, B. L.; Zacharias, M., *Front Chem*, **2020**, *8*, 573259.

PP 15

Natural Phytochemicals from Simaroubaceae family as SARS-Cov-2 M Pro inhibitors: A Computational Molecular Docking and Simulation Approach

Athira E[a], Vijisha K. Rajan[a,*]

[a]*Department of Nanoscience and Technology, University of Calicut, Malappuram-673635,*
**drvijishakrajan@uoc.ac.in*

Keywords: SARS-CoV-2, M Pro, Molecular docking, Molecular Dynamics (MD) simulations, ADMET

In the battle against infectious diseases, COVID 19 has been a tough opponent. COVID-19, also known as Coronavirus Disease 2019, is a highly contagious respiratory illness caused by the SARS-CoV-2 virus, initially identified in Wuhan, China in late 2019. A promising approach to combat the SARS-CoV-2 pandemic involves the development of novel, targeted medications that inhibit essential viral proteins. Computer-aided drug design is a game-changer for researchers looking to develop new COVID-19 treatments, offering a faster and more efficient alternative to traditional methods. The M Pro enzyme, essential for SARS-CoV-2 replication, has been identified as a key target for the design of COVID-19 inhibitors. Inhibition of M Pro's proteolytic activity presents an optimal therapeutic approach to impede the replication of SARS-CoV-2 within host cells. Plant-derived phytochemicals, renowned for their prophylactic properties against various diseases, including viral infections, have been identified as potent inhibitors of SARS-CoV-2 M Pro, exhibiting promise as antiviral agents. Quassinoids - a group of oxygenated triterpenoids from the simaroubacea plant family exhibit a broad spectrum of biological activities like anticancer, antimalarial, antiviral, and anti-inflammatory activities. In this study, we undertook a comprehensive investigation to assess the inhibitory potential of 18 Quassinoids against M Pro, employing a multi-faceted approach that integrated molecular docking studies, Molecular Dynamics (MD) simulations, MM-GBSA analysis, and ADMET analysis. This investigation presents Gutolanthone as a highly potent inhibitor of M Pro, surpassing the efficacy of Molnupiravir. Additionally, gutolanthone demonstrated a superior safety profile, marked by minimal toxicity and maximal biocompatibility.

References

1. Ahmad, A.; Kaleem, M., *Food Res. Int.*, **2015**, *77*, 221–235.
2. Zheng, J., *Int J Biol Sci*, **2020**, *16*, 1678–1685.
3. Cucinotta, D.; Vanelli, *M., Acta Bio-Medica: Atenei Parmensis*, **2020,** *91*, 157–160.

PP 16

Sustainable Synthesis of Reduced Graphene Oxide *via* Phyto Extracts- Assisted Hydrothermal Method for Environmental Photocatalysis

Adithi N[a], G. K. Nagaraja[a,*]
[a]*Department of Chemistry, Mangalore University, Mangalagangothri, Mangalore, Karnataka, India*
[*]*nagarajagk@gmail.com*

Keywords: Reduced graphene oxides, Hydrothermal method, Phyto extracts, Physicochemical property, Photo catalyst.

Nowadays, for environmental remediation, photocatalytic process involving graphene-based semiconductors is considered a very promising oxidation process for water treatment. The remediation of persistent organic pollutants in water demands the development of efficient, sustainable, and eco-friendly catalytic materials. This study reports the successful green synthesis of highly fluorescent Graphene Quantum Dots (GQDs) using a simple, scalable hydrothermal method, leveraging a readily available and non-toxic biomass precursor as the sole carbon source. The synthesized GQDs were extensively characterized using high-resolution transmission electron microscopy, X-ray diffraction, and photoluminescence spectroscopy, Raman spectroscopy confirming their uniform nanoscale dimensions and desirable optical properties. The primary objective was to evaluate the photocatalytic performance of these green-synthesized GQDs against a model organic pollutants, under simulated solar irradiation. The GQD catalyst exhibited exceptional efficiency, kinetic analysis confirmed that the degradation process followed a pseudo-first-order model, highlighting the high reactivity of the material. This significantly enhanced performance is attributed to the GQDs' unique quantum confinement effects, which promote superior generation of reactive oxygen species and inhibit the recombination of photo- generated electron-hole pairs. The results revealed that the catalytic efficiency varied depending on the type of phytoextract used, due to differences in surface functional groups, particle size, and degree of reduction. Among the tested samples, the rGO with optimal surface properties exhibited superior degradation efficiency and reusability. This comparative study highlights the potential of phyto-mediated rGO as an effective and sustainable photocatalyst for environmental remediation and wastewater treatment applications.

References

1. Raja, A.; Rajasekaran, P.; Selvakumar, K.; Arivanandhan, M.; Asath Bahadur, S.; Swaminathan, M. *Optik* **2019**, *190*, 21–27.

2. Parthipan, P.; Cheng, L.; Rajasekar, A.; Govarthanan, M.; Subramania, *Environ. Res.* **2021**, *196*, 110983.

PP 17

Efficient Photocatalytic Degradation of Methylene Blue Dye using Brookite TiO_2/N-Doped Graphene Nanocomposite under UV Irradiation

Amritha C. Jayasankar[a], Mohamed Haseen K. P.[b], Muhsina P. P.[b], Binitha N. Narayanan[a,*]

[a]*Department of Chemistry, University of Calicut, Malappuram, India*
[b]*Department of Chemistry, Markaz Arts & Science College, Karthala, Athavanad*
[*]*binithann@uoc.ac.in*

Keywords: TiO_2/N-doped Graphene, Photocatalyst, Dye degradation.

A Brookite-phase TiO_2/N-doped graphene nanocomposite(TiO_2/NG) was synthesized via a simple sol–gel and hydrothermal method and evaluated for photocatalytic degradation of methylene blue (MB) under UV light. Brookite TiO_2, though less studied, offers superior photocatalytic activity due to efficient charge separation and favorable conduction band alignment. Its formation under mild conditions enhances scalability. Nitrogen-doped graphene (NG) improves light absorption, provides active sites, and facilitates charge transport, reducing recombination. Characterization using XRD, FTIR, UV-Vis DRS, SEM, TEM, and XPS confirmed successful synthesis and N-doping. The nanocomposite showed excellent MB degradation, highlighting the synergistic interaction between Brookite TiO_2 and NG. This study demonstrates a cost-effective approach to developing efficient photocatalysts for environmental applications.

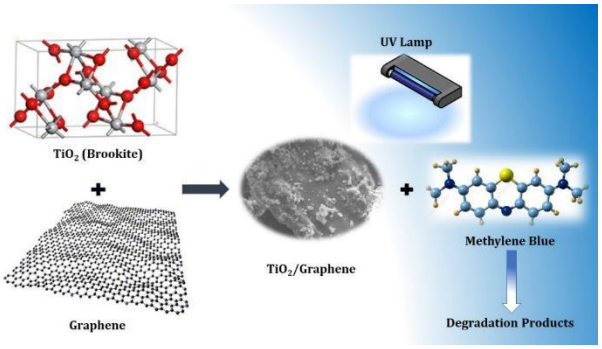


Figure 1: Graphical Abstract of Methylene Blue Degradation

References

1. Gupta, V. K.; Pathania, D.; Agarwal, S.; Singh, P., *J. Hazard. Mater.*, **2012**, *243*, 179–186.
2. Li, R.; Li, Q.; Zong, L.; Wang, X.; Yang, J., *Electrochimica Acta*, **2013**, *91*, 30–35.

PP 18

Synthesis and Characterizations of Graphene Oxide Modified Cerium Nano Composite

Anjali C[a,*], Renuka N. K[b], Archana M. S.[a], Ashima, Archana N. K[a], Arya Shaji P[a], Aswinesh K[a]

[a]*Department of Chemistry, St. Joseph's College (Autonomous), Devagiri, Calicut, Kerala-673008, India*

[b]*Advanced Materials Research Centre, Department of Chemistry, University of Calicut, Kerala-673 635, India*

**anjalibaburajan7@gmail.com*

Keywords: Graphene oxide, Cerium nano composite, Humidity sensing Electrochemical devices.

Metal oxides play a vital role in environmental remediation and pollutant detection and hold strategic importance in various other sectors such as energy generation, conversion, and storage. Their wide range of functional properties is strongly influenced by factors including crystal structure, morphology, composition and doping, which in turn govern their optical, electrical, chemical, and catalytic behaviors. Among these, rare earth metal oxides and their composites have gained significant attention due to their environmentally friendly nature, cost-effectiveness, and scalability. Within this category, cerium oxide (CeO_2) is of particular interest. Cerium, a rare earth element and the second member of the lanthanide series, is one of the most abundant rare earth metals in Earth's crust, occurring at approximately 66 ppm in its metallic and oxide forms[1,2].

Cerium oxide nanoparticles (CNPs) find applications in advanced technologies such as solid oxide fuel cells, high-temperature oxidation protection coatings, catalysts, oxygen sensors, and solar cells. However, to further enhance their performance for additional applications such as humidity sensing and electrochemical devices property optimization is necessary. In this work, we aim to modify rare earth oxides by incorporating graphene, a remarkable material known for its outstanding functional properties [4,]. Instead of pure graphene, graphene oxide (GO) is employed owing to its ease of handling and compatibility with various compounds. The study also explores how the mutual interaction between rare earth oxides and graphene oxide enhances the properties of both materials. The resulting graphene oxide–modified cerium oxide composites were thoroughly characterized using various analytical techniques, including FT-IR, XRD, FE-SEM, HR-TEM, BET, and UV–DR spectroscopy. The results confirm the successful formation of the graphene oxide–modified cerium composite.

References

1. Ansari, S. A.; Khan, M. M.; Ansari, M. O.; Kalathil, S.; Lee, J.; Cho, M. H. *RSC Adv.*, **2014**, *4*, 16782-16791
2. Ansari, A. A. *J. Semicond.*, **2010,** *31*, 053001.

PP 19

Synthesis, Characterization and Applications of CTAB Modified Organo Clay for Pb(II) Adsorption

Anjali R Mohan[a], *Sneha S* [a], *Bency John* [a,*]
[a]*Department of chemistry, SG College Kottarakara, Kollam - 691531, Kerala, India*
[*]*bencyjohn136@gmail.com*

Key words: Montmorillonite clay, Adsorbent, Characterization, Adsorption kinetics, Pb (II) removal

In the present work, a surfactant-modified organoclay was synthesized and used as an efficient adsorbent for the removal of Pb(II) ions from aqueous solution. Sodium montmorillonite (Na-MMT) was chosen as the base clay and modified with the cationic surfactant cetyltrimethylammonium bromide (CTAB) and humic acid (HA). The modification was confirmed through FTIR, SEM, TGA, XRD, and BET analyses, which revealed structural and surface property enhancements, including increased surface area and improved adsorption potential. Batch adsorption experiments were performed to investigate the influence of pH, contact time, temperature, and initial metal ion concentration. The results showed that the adsorption efficiency increased with pH and reached a maximum of 92.23% at pH 5 and an initial Pb (II) concentration of 10 mg/L [1]. The equilibrium data were best fitted to the Freundlich isotherm model ($R^2 = 0.9963$), suggesting multilayer adsorption on a heterogeneous surface, whereas the Langmuir model ($R^2 = 0.975$) showed a slightly lower correlation [2] . Kinetic studies demonstrated that the pseudo-second-order model ($R^2 = 0.991$) provided the best fit, indicating chemisorption as the rate-controlling step. The adsorption of Pb(II) onto the modified clay was spontaneous and endothermic, with $\Delta H° = 65.96$ kJ/mol and $\Delta S° = 206.62$ J/K·mol, indicating increased randomness at the solid–liquid interface and strong interactions between Pb(II) ions and the clay surface. Overall, Pb(II) removal using CTAB/HA-modified Na-MMT was spontaneous and endothermic, confirming its effectiveness as a sustainable and eco-friendly adsorbent.

References

1. Baghdadi, M.; Mazarji, M.; Sabouhi, M.; Kang, A. J.; Jafari, A., *J. Adv. Chem.* **2014**, *9*, 2062-2071.
2. Anjum, A.; Ansar, P.; Punnuswamy Lokeswari; Kaur, M.; Datta, M., *J. Anal. Sci. Methods Instrum.* **2011**, 1, 25-30.

PP 20

Tailoring BiSI Chalcohalides for Enhanced Semiconductor-Sensitized Solar Cell Applications

Anna Mariya Thomas[a], Subila K. B.[a,*]

[a]*School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala, India.*
**subilakb@mgu.ac.in*

Keywords: Chalcohalides, Bandgap tuneability, Lead-free, Semiconductor-sensitized.

The need for environmentally benign, thermally stable, and lead-free semiconductors has driven interest in chalcohalides.[1,2] Among these, bismuth sulfoiodide (BiSI) offers an optimal band gap, strong light absorption and robust stability, making it a promising candidate for photovoltaic and optoelectronic devices.[3,4,5] In this work, Bismuth sulfoiodide (BiSI) was synthesised using both hydrothermal and microwave-assisted methods by varying iodine content. X-ray diffraction (XRD) revealed that the microwave route produced highly crystalline, orthorhombic, phase-pure BiSI, while the hydrothermal method yielded mixed phases. FESEM images showed uniform rod-like morphologies, and UV-Vis spectroscopy indicated strong absorption ($\lambda\_max \approx$ 693- 702 nm) with band gaps tunable from 1.26 to 1.44 eV. Raman spectra confirmed structural integrity, and TGA demonstrated thermal stability up to ~343 °C.

A mechanistic study of the $Bi_2S_3 \rightarrow$ BiSI transformation revealed that microwave synthesis promotes rapid and uniform heating, enabling homogeneous nucleation and fast iodine incorporation into the Bi–S lattice. This suppresses intermediate phase formation and drives the system towards the thermodynamically stable orthorhombic phase. In contrast, slower, non- uniform heating in hydrothermal synthesis leads to incomplete reactions and metastable S-rich intermediates. The superior phase purity, faster reaction time and lower processing temperature achieved via the microwave approach underscore its potential as a scalable route for high-quality, lead-free BiSI in next-generation optoelectronic devices.

References

1. Sun, H.; Yang, G., *J. Mater. Chem. C*, **2020**, *8*, 13253–13262.
2. Tiwari, D.; Alibhai, D., *ACS Appl. Energy Mater.*, **2019**, *2*, 3878–3885.
3. Mombrú Frutos, M.; Grosso, C., *Inorg. Chem.*, **2022**, *61*, 9231–9240.
4. Li, S.; Xu, L.; Kong, X., *J. Mater. Chem. C*, **2020**, *8*, 3821–3829.
5. Zhao G.; Mei B., *Inorg. Chem.*, **2024**, *63*, 3460−3466.

PP 21

Exploring a Benzimidazole Linked Covalent Triazine Framework System for High-Performance Fluorescent Detection of Trinitrophenol

Anna Merin Joy[a], Dr. Kala R[a,*]

[a]*Department of Applied Chemistry, Cochin University of Science and Technology, Kalamassery*

[*]*kala@cusat.ac.in*

Keywords: Covalent triazine framework, Trinitrophenol (TNP), Fluorescent sensing.

Nitroaromatic compounds play a significant role in diverse applications, including dyes, rocket fuels, and military explosives. However, their persistence in the environment, coupled with their high toxicity, has raised concerns, prompting researchers to develop efficient detection strategies. Among these compounds, trinitrophenol (TNP), is of particular interest due to its high-water solubility, explosive nature, and severe health hazards, posing risks not only to humans but also to ecosystems.[1,2] Hence, the selective and sensitive detection of TNP is crucial. While various analytical techniques exist, fluorescence-based sensing is highly advantageous due to its exceptional sensitivity, selectivity, real-time monitoring capabilities, and ease of operation.[3]

Covalent Triazine Frameworks (CTFs), a subclass of porous organic polymers, have emerged as promising materials for fluorescent sensing due to their porosity, heteroatom incorporation potential, and extended conjugation.[4] In this study, a benzimidazole-linked Covalent Triazine Framework ($CTF_{TFPOT\text{-}BTA}$) was synthesized and further characterized using PXRD, FTIR,TGA, UV Visible spectroscopy etc. and employed as a fluorescent sensing platform for TNP detection. The sensing mechanism involves the interaction between TNP and the electron-rich framework, leading to fluorescence quenching. This interaction enables ultra-trace detection of TNP with an excellent LOD 1.38 nM, making the material highly suitable for environmental monitoring and security applications.

Driven by the vision of achieving multi-platform detection, we have successfully fabricated a CTF-$_{TFPOT\text{-}BTA}$ film by embedding the framework within a PVA matrix, thereby extending its functionality beyond conventional suspension-based sensing. The developed film demonstrates exceptional sensitivity toward trinitrophenol (TNP)**,** along with remarkable photostability**,** excellent reusability**,** and outstanding potential for real-time monitoring**.** To further translate this laboratory success into practical application, a portable sensing device was indigenously

engineered, enabling rapid, on-site, and user-friendly detection of TNP**.** This advancement not only underscores the versatility and robustness of the material but also establishes it as a promising candidate for real-world environmental and security monitoring systems.

References

1. Kaja, S.; Damera, D. P.; Nag, A., *Analytica chimica acta,* **2020**, *1129*, 12–23.
2. Nath, S.; Pathak, S. K.; Pradhan, B.; Gupta, R. K.; Reddy, K. A.; Krishnamoorthy, G.; Achalkumar, A. S., *New J. Chem.,* **2018**, *42* , 5382–5394.
3. Vijayan, A. P.; Ramakrishnan, K.; Elambalassery, J. G., *ACS Appl. Polym. Mater.,* **2024**, *6* , 3975–3984.
4. Liao, L.; Li, M.; Yin, Y.; Chen, J.; Zhong, Q.; Du, R.; Liu, S.; He, Y.; Fu, W.; Zeng, F., *ACS Omega. American,* **2023,** *8*, 4527–4542.

PP 22

Synthesis of Pd-Integrated Carbon Dot@TiO_2 Thin Film for Photocatalytic Glycerol Reforming Reaction for Producing Hydrogen

Athira Abraham,[a] Kranti N. Salgaonkar, [a,b] Chinnakonda S. Gopinath, [a,b] and Avishek Saha[a,b,*]

[a]*Catalysis and Inorganic Chemistry Division, CSIR-National Chemical Laboratory, Dr Homi Bhabha Road, Pune 411008, India*

[b]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India*

** avi.saha@ncl.res.in*

Keywords: Water splitting, Biomass component, Organic valorisation, Energy conversion

Hydrogen is widely acknowledged as a crucial energy carrier for a sustainable future due to its high gravimetric energy density (141.9 MJ/kg) than any conventional fossil fuels along with zero carbon emissions when used as a fuel.[1,2] As the demand for clean energy is increasing, the development of sustainable hydrogen production methods has become a major focus in research areas, especially in energy conversion and storage using renewable energy, such as solar energy, wind energy, etc.[3] Due to low cost, non-toxicity, and stability of titanium dioxide (TiO_2), it is widely used for H_2 production. In order to improve the activity, TiO_2 can be modified by doping, morphology control, heterojunction formation with metal/semiconductor clusters, and surface modification strategies. In the past decade, many researchers have reported the application of carbon dot (CD) in photocatalytic overall water splitting (OWS). Replacing the kinetically sluggish oxygen evolution reaction (OER) with the oxidation of an abundantly available organic molecule to value-added product(s) (VAPs) at low voltage along with the hydrogen evolution reaction (HER)is a big challenge in water splitting. Glycerol, a low-cost and abundant byproduct of the biodiesel industry, is particularly attractive as a sacrificial agent due to its multiple hydroxyl groups. Glycerol oxidation to a VAP is kinetically fast, compared to an OER, and offers hope to enhance sunlight-driven water splitting to hydrogen by the concurrent utilization of holes and electrons.[4,5] A series of thin-film photocatalysts comprising TiO_2 modified with carbon dots (CDs) dispersed either with palladium (Pd-CD/TiO_2) or nickel (Ni-CD/TiO_2) were synthesized via solid-state and wet-impregnation methods. Under direct sunlight illumination, Pd-CD/TiO_2 thin film exhibited superior hydrogen yield and maintained stability over 25 h, outperforming Ni-CD/TiO_2 and bare TiO_2 photocatalyst thin films. Concurrent glycerol oxidation at neutral pH (pH~7) yields glycolaldehyde, formic acid, and dihydroxyacetone as VAPs. Enhanced photocurrent density and lower impedance of Pd-CD/TiO_2

corroborate improved charge carrier separation and dynamics. The results demonstrate that Pd-CD synergistically improve the photocatalytic performance of the Pd-CD/TiO_2 for sustainable hydrogen generation and selective biomass valorisation.

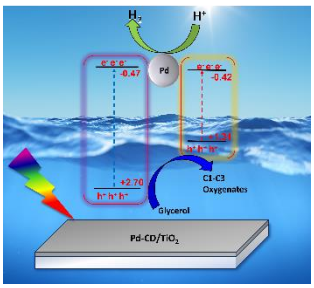


Figure 1. Possible mechanism for Pd-CD/TiO2 toward photocatalytic hydrogen generation and glycerol oxidation toward value-added products

References

1. Nalajala, N., Patra, K. K., Bharad, P. A. & Gopinath, C. S. *RSC Adv.* **2019** ,*9*, 6094–6100.
2. Atwater, H. A. *Phys. Today*, **2023** ,*76*, 32–39
3. Rajaambal, S., Sivaranjani, K. & Gopinath, C. S. *J. Chem. Sci.* ,**2015**. *127*, 33–47.
4. Bajpai, H., Chauhan, I., Salgaonkar, K., Mhamane, N. B. & Gopinath, C. S. *RSC Sustain.*,**2023** *1(3)*, 481-493
5. Nivedhitha, T. R. *et al. ACS Sustain. Chem. Eng.*,**2024**, *12(40*), 14841-14853.

PP 23

Correlation of Physiochemical Properties with Dyedegradation Using Reduced Graphene Oxide Prepared from Phytoextract by Green Synthesis

Bhagyalakshmi. P[a], Sanjay Annarao[a,*], Adithi N[b]

[a]*Department of PG Chemistry, University College Hampanakatta, Mangalore, Karnataka, India*

[b]*Department of Chemistry, Mangalore University, Mangalagangothri, Mangalore, Karnataka, India*

[*] *Sanjaymulge@gmail.com*

Keywords: Phytoextract, Physiochemical properties, Dye degradation, Morphology.

The disposal of untreated textile industrial wastewater having unmanageable pollutants is a global issue. Eco-friendly remediation technology is needed for the removal of environmental contaminants. Industrial dye effluents represent a major environmental concern due to their chemical stability and resistance to biodegradation. In this study, reduced graphene oxide (rGO) was synthesized using a phytoextract-based green synthesis approach, offering an eco-friendly alternative to conventional chemical reduction. The prepared rGO was then utilized as a photocatalyst for the degradation of synthetic dye solutions under solar insolation. To evaluate the progress of degradation, various physicochemical parameters such as turbidity, surface tension, and viscosity were systematically monitored. A gradual decrease in turbidity and viscosity accompanied by an increase in surface tension indicated the breakdown of large dye molecules into smaller, less surface-active intermediates. The correlation of these parameters with UV–Vis spectroscopic data confirmed efficient photocatalytic activity of the green- synthesized rGO. The study demonstrates that simple physicochemical measurements can effectively reflect dye degradation behavior and highlights the potential of plant-extract-mediated rGO as a sustainable and cost-effective photocatalyst for wastewater treatment applications.

References

1. Lee, G.; Kim, B. S., *Biotechnol. Prog.* **2014**, *30*, 463–469.
2. Zaaba, N. I.; Foo, K. L.; Hashim, U.; Tan, S.J.; Liu, W.W.; Voon, C.H., *Procedia Eng.* **2017**, *184*, 469–477.

PP 24

A Detailed Study of Spinel Ferrites as Gas Sensors for Toxic Gases

K Ahalya[a], **Binila K**[b*],
[a] *The Zamorins Guruvayurappan College, Calicut*
[b]*The Malabar Christian College, Calicut*
[*]*binila2222@gmail.com*

Keywords: Magnetic nanoparticles, Ferrites, Gas sensors, Sensors, Iron oxide

Gas sensors play a vital role in monitoring toxic and flammable gases, with growing importance in environmental protection, industrial safety, and healthcare. Recent advances in nanostructured ferrite materials have created opportunities for developing low-cost, efficient, and highly sensitive gas sensors. Among them, copper ferrite ($CuFe_2O_4$) and nickel ferrite ($NiFe_2O_4$) nanoparticles are promising candidates due to their stable spinel structure, good chemical stability, and excellent magnetic and electrical properties. Their nanoscale dimensions provide a high surface-to-volume ratio, enabling enhanced interaction with gas molecules and improved sensing performance. In this work, $CuFe_2O_4$ and $NiFe_2O_4$ nanoparticles are employed in the fabrication of simple pellet-based gas sensors. A self-designed gas sensing apparatus will be used to evaluate their response towards hazardous gases such as ammonia (NH_3) and methanol (CH_3OH). The sensing mechanism is based on the change in electrical resistance of the ferrite pellets upon exposure to test gases, caused by surface adsorption and redox reactions at the gas–solid interface. The sensor performance is studied systematically in terms of sensitivity, response, and recovery times, reproducibility, and selectivity. To understand the factors affecting sensing behaviour, samples synthesized under different pH values and sintering temperatures are compared. Variations in sensing performance are correlated with structural, morphological, and magnetic differences of the ferrites. The dependence of sensor response on gas concentration, operating temperature, and desorption behaviour is also analysed in detail. This study aims to demonstrate that ferrite nanoparticles can serve as efficient, low-cost sensing materials for the detection of toxic and flammable gases. By establishing clear relationships between synthesis conditions and sensing performance, the work highlights the potential of $CuFe_2O_4$ and $NiFe_2O_4$-based sensors for applications in environmental monitoring, industrial safety systems, and future smart sensing technologies.

References

1. Wang, X.L.; Gong, D.; Zhang, X., *Sens. Actuators B.Chem.,* **2020***, 322,* 128616.
2. Ranjith Kumar, E. *et al*. *Sens. Actuators B.Chem,* **2014,** *191*, 186-191.

PP 25

Evaluating the Preferential Adsorption of N_2 from a Binary Mixture of N_2/O_2 on Extra-Framework Cations of Zeolites: A Computational and Experimental Study

George Devasia[a,c], Sachin Nandanwar[b], Sailaja Krishnamurty[a,c*]

[a]*Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Pune, India*

[b]*Catalysis and Inorganic Chemistry Division, CSIR-National Chemical Laboratory, Pune, India*

[c] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India*

[*]*sailaja.raaj@gmail.com*

Keywords : Zeolites, N_2/O_2 separation, Molecular dynamics.

Separation of N_2 from a N_2/O_2 gas mixture is critical for various industrial/medical applications. Temperature/pressure swing adsorption is the top-notch industrial technology used for this separation, where zeolites are the materials used for adsorption.[1] Zeolite X/Y with Li^+ as an extra-framework cation is the best-known sorbent for N_2 gas molecules. However, the present net-zero emission scenario has made lithium a critical element, making it imperative to implement its alternative in various other technologies. In this context, the present work is a computational evaluation to identify a cation that can replace Li^+ for preferential adsorption of N_2 over O_2. The DFT study, based on parameters such as selective adsorption energies of N_2 over O_2 and IR stretching frequencies of the adsorbed N_2 and O_2 molecules, identifies Mg^{2+}, Ca^{2+}, Sr^{2+}, Co^{2+} and Zn^{2+} as potential cations. These cations have preferential adsorption for N_2 over O_2 by 10 kJ mol^{-1} or more. However, BOMD simulations reveal that only Mg^{2+}, Ca^{2+}, Co^{2+} and Zn^{2+} keep the N_2 molecule bound at 300 K, and the O_2 molecule gets desorbed from these frameworks. The desorption temperature of N_2 on Ca^{2+} and Zn^{2+} is 350 K, and on Mg^{2+} is 400 K. These observations are corroborated by electronic charges on cations and molecular orbitals. Significantly, Ca^{2+} is identified to adsorb up to 2 N_2 molecules, making it an ideal candidate for N_2/O_2 separation in place of Li^+. To validate this, we have carried out an experimental study that showed a good N_2 adsorption capacity of 2.1 mmol g^{-1} for Ca^{2+}.[2]

References

1. E. Pérez-Botella.; S. Valencia.; F. Rey., *Chem. Rev.*, **2022**, *122*, 17647.
2. G. Devasia.; S. Nandanwar,; S. Krishnamurty., *Phys. Chem. Chem. Phys.*, **2025**, *27*, 7846.

PP 26

Novel Nb_2C Mxene/Polypyrrole Composite Synthesized *via* Cerium-Mediated Bi-Solvent Route for High Performance Electrochemical Biosensing

Haneena K P[a], Mini Mol Menaparambath[a,*]

[a]*Laboratory for Advanced Materials and Applied Research, Department of Chemistry, National Institute of Technology, Calicut, Kerala, 673-601*

**minimol@nitc.ac.in*

Keywords: Mxene, Polymer composites, Bi solvent Synthesis, Tyrosine sensing

Niobium carbide (Nb_2C) MXene, a member of the two-dimensional transition metal carbide family, has recently emerged as a promising material owing to its high metallic conductivity, hydrophilicity, and tunable surface terminations. These properties make Nb_2C particularly attractive for electrochemical applications such as energy storage and biosensing. However, issues like sheet restacking and limited surface reactivity often restrict its practical performance. Surface modification through conducting polymer incorporation offers an effective strategy to overcome these limitations by improving interlayer spacing, introducing additional redox-active sites, and enhancing overall stability and charge transport.[1] In this work, a bi-solvent (hexane/water) assisted polymerization strategy was employed to synthesize a novel Nb_2C MXene/polypyrrole (PPy) composite using cerium nitrate as a mild oxidizing agent. The dual solvent system promoted uniform pyrrole dispersion and homogeneous polymer growth on the MXene surface,[2] while cerium ions served both as oxidant and redox-active dopant. Successful modification of Nb_2C was confirmed through SEM, XRD, and Raman analyses, which revealed uniform PPy coating and strong interfacial interaction. The resulting Nb_2C/PPy–Ce composite exhibited excellent electrocatalytic activity toward *L*-tyrosine detection, an essential biomarker related to neurological and metabolic disorders such as Parkinson's disease, schizophrenia, and phenylketonuria. The superior sensing performance originates from the synergistic interplay between the conductive Nb_2C framework and the redox-active PPy–Ce interface. This study presents a simple and efficient cerium-assisted, bi-solvent polymerization route for developing high-performance MXene-based electrochemical biosensors.

References

1. Kumar S, Zain Mehdi SM, Taunk M, et al. *J Mater Chem A*. **2025,** *13*,11050-11113.
2. Sugunan A, Anil Syamala A, Radhakrishnan AB, Menamparambath MM. *Nanoscale Adv*. **2025**, *7*,4980-4993.

PP 27

$ScCO_2$-Mediated Morphological Engineering for Controlled-Release Formulations of Metoprolol Tartrate

Hanna Ameena M A[a,*], Poovathinthodiyil Raveendran[a]
[a]*Department of Chemistry, University of Calicut, Thenhipalam, India*
**hannaameenama@gmail.com*

Keywords: Supercritical CO_2, Solid dispersion, Controlled drug release, Bioavailability, Morphology.

Supercritical CO_2 -technology has been utilized to prepare solid dispersions (SD) of Ibuprofen (IBU) in excipient matrices of hydrophilic polyethylene glycol (PEG) and hydrophobic sucrose octaacetate (SOA). The single-step process involves magnetic stirring of the drug and the excipients at 35 °C and 90 bars in $scCO_2$ for an hour to obtain the final composite. $ScCO_2$, being a cheap, abundant, non-toxic, and non-flammable solvent with a low critical point (T_c = 31.1 °C, P_c = 73.8 bar), makes the process simple, efficient, and environmentally benign. At the end of the process, depressurization removed the CO_2 completely, leaving no residual solvents behind. The resulting composites had distinct structural and morphological features, which could be attributed to the peculiar solvent effects of $scCO_2$ on the excipients. Further, the uniqueness of this solvent system was validated by comparing the properties of similar composites prepared using acetone, a conventional organic solvent. Both the composites had a controlled-release profile. The composites exhibited no significant changes in release profile even after a few months, suggesting potential applications of this method in the pharmaceutical industry.

References

1. Raveendran, P.; Ikushima, Y.; Wallen, S. L.; *Acc. Chem. Res.*, **2005**, *38*, 6, 478–485.
2. Ramachandran, J. P. et al.; *J.CO_2. Util.*, **2021**, *47*, 101472.

PP 28

From Aluminum to Indium: Linking Porphyrin Structure to Electrochemistry for Artificial Photosynthesis

Haritha Anamangattupurakkal[a], Arifa Kaniyantavida[a], Jayachandran Kaippully[a], Aparna Chencharodi[a], Sajimon[a], Sebastian Nybin Remello[b], Hiroshi Tachibana[c], Haruo Inoue[c], Fazalurahman Kuttassery[a*]

[a] *Department of Chemistry, University of Calicut, Malappuram 673635, Kerala, India*

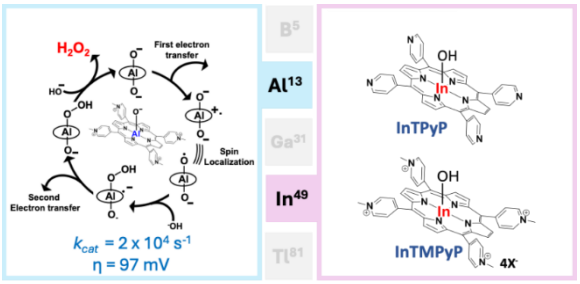
[b]*Department of Applied Chemistry, Cochin University of Science and Technology, Kochi 682022, Kerala, India*

[c]*Department of Applied Chemistry for Environment, Graduate School of Urban Environmental Sciences, Tokyo Metropolitan University, 1-1 Minami Osawa, Hachioji, Tokyo, 192-0397, Japan*

[*] *kfazalurahman@uoc.ac.in*

Keywords: Artificial photosynthesis, Molecular-material hybrid systems, Indium-porphyrins.

The development of clean technologies for converting solar energy into chemical fuels offers a promising route to address global energy and environmental challenges. Among these, solar-driven two-electron water oxidation to hydrogen peroxide provides a sustainable alternative to conventional industrial processes, minimizing carbon emissions and environmental impact. Porphyrin-based photocatalysts, with their broad visible-light absorption, represent an attractive platform for such reactions. While main-group metalloporphyrins incorporating Al^{3+}, Si^{4+}, Ge^{4+}, and Sn^{4+} have been extensively explored, indium porphyrins remain largely unstudied. Here, we report the synthesis and characterization of two indium(III) porphyrins—5,10,15,20-tetrakis(4-pyridyl)porphyrinate indium(III) (InTPyP) and its N-methylated analogue, 5,10,15,20-tetrakis(N-methyl-4′-pyridiniumyl)porphyrinate indium(III) (InTMPyP). Designed as structural analogues of aluminum porphyrins, these complexes were systematically investigated to compare their electronic, photophysical, and photocatalytic properties. Our findings highlight the potential of indium-based porphyrins as promising candidates for solar-driven artificial photosynthetic devices.



Scheme1: Overview of the molecular mechanism for oxidative H_2O_2 formation from water catalyzed by AlTMPyP electrocatalyst under homogeneous conditions (left), and molecular structures of indium porphyrins (InTPyP and InTMPyP) designed for the present study (right).

References

1. Kuttassery, F.; Mathew, S.; Sagawa, S.; Remello, S.N.; Thomas, A.; Yamamoto, D.; Onuki, S., Nabetani, Y.; Tachibana, H.; Inoue, H., *ChemSusChem*, **2017**, *10*, 1909-1915.
2. Guo, Y.; Zhou, Q.; Wang, L.; Deng, Z.; Phillips, D.L.; Tang, C.Y.; Zhu, Y., *Nature Commun.*, **2025**, *16*, 6297.

PP 29

Catalytic Revolution in Iron-Making: Catalyst Materials for Various Blast Furnace Feed-Stocks for Sustainable Iron Making

Omkar G Kavade[a], Ritul Mishra[a], Santosh Kumar Sriramoju[a,*]
[a]*Chemical Engineering & Process Development Division, CSIR-National Chemical Laboratory, Pune, India.*
[*]*sk.sriramoju.ncl@csir.res.in*

Keywords: Blast furnace feedstocks, **Catalytic iron-making**, **Metal oxide catalysts**, **Coke oven efficiency**.

The blast furnace route remains the dominant iron-making process, accounting for nearly 70% of the world's steel production**.** Indian steel plants produce ~160 million tonnes of hot metalannually through blast furnaces, consuming an average of 450–550 kg of coke, 150–200 kg of pulverized coal injection (PCI), and 1.5–1.6 tonnes of iron-bearing materials (sinter, pellets, and lump ore) per tonne of hot metal. This conventional route contributes approximately 1.8–2.1 tonnes of CO_2 per tonne of hot metal, making the iron and steel sector responsible for nearly 7–9% of total anthropogenic CO_2 emissions. Feedstock preparation itself is highly energy-intensive. Coke ovens operate at around 1100–1200°C, consuming about 400–450 kg of coal per tonne of coke produced (with a thermal efficiency below 40%), while sintering of fine ores at 1300–1400°C consumes 50–60 kg of coke breeze and 7–8 GJ of energy per tonne of sinter. Thus, improving the energy efficiency and reactivity of these feedstocks can directly enhance blast furnace performance and lower emissions.

This research aims to develop catalytic materials and process interventions that accelerate sintering reactions and improve coke oven conversion, thereby reducing fuel consumption and increasing plant productivity. Carbonaceous materials can oxidize more quickly and completely when metal oxide-based catalyst materials improve coal combustion kinetics and reduce activation energy barriers.[1,2] The prepared catalyst shows a reduction of coking time by 6% without impacting coke CSR, CRI, and cold strength properties. Prepared catalyst reduces the energy barrier for coal fluidization reactions, allowing devolatilization to occur more efficiently at lower temperatures. Furthermore, the catalyst helped improve the heat transfer rate within the coal cake. These catalysts enhance oxygen transport and increase heat transfer efficiency inside coal particles, leading to enhanced devolatilization at reduced temperatures.[3]

Different catalyst materials were prepared and tested for sinter making and it was found that, magnesium based metal oxide coated on an activated carbon substrate shows better performance.[4] The coke breeze deformation temperature and sinter

deformation temperatures were reduced by ~100ºC with the use of the catalyst. This shows that, the use of catalyst reduces the deformation temperature, so that the reactivity of coke breeze can start at lower temperatures and thereby activation energy required for sinter deformation reduces. The reduction in sinter deformation temperature led to a reduction in sintering time and, therefore, sinter plant productivity will increase without any capacity enhancement.

References

1. Wang, R.; Zhang, J.; Xu, R.; Wang, L.; Zhu, Q.; Zeng, Y.; Zhang, N.; Huang, X., *Energy*, **2025**, *321*, 135103.
2. Cao Y.; Xiao, J.; Lv, Y.; Tang, S.; Wen, L.; Tang, W., *Fuel*, **2024**, *358*, 130126.
3. Zhang, H.; Dou, B.; Li, J.; Zhao L.; Wu, K., *J. Energy Inst.*, **2020**, *93*, 2526.
4. Vega, M. F.; Díaz-Faes, E.; Barriocanal, C., *ACS Omega*, **2021**, *6*, 34615.

PP 30

A Novel Naphthalimide-TREN-based Schiff Base for Selective Detection of Zn(II) Ions using the ESIPT Mechanism

Ruhila Taj Mehboob Ali[a], Noushija Mannanthara Kunhumon[b], and Sankarasekaran Shanmugaraju[a,*]

[a]*Department of Chemistry, Indian Institute of Technology Palakkad (IIT PKD), Palakkad, Kerala, India.*

**202414007@smail.iitpkd.ac.in*

Keywords: Napthalimide-TREN-based schiff base, One-pot synthesis, ESIPT mechanism, Zinc ion detection at the ppm level.

Zinc, the second most abundant metal ion in the human body, plays a vital role in numerous catalytic and biological processes.[1] However, fluctuations in its concentration within biological systems and the environment can pose significant health risks,[2,3] highlighting the need for a less toxic and highly efficient zinc-detecting compound. In this study, a Naphthalimide-TREN-based moiety was selected owing to its excellent photostability, structural flexibility, and ease of synthesis. Using a one-pot synthetic route, we successfully developed and fully characterised a Naphthalimide-TREN-based Schiff base derivative (NapSB). Spectroscopic investigations using UV-Visible and fluorescence techniques confirmed that NapSB exhibits selective and reversible binding toward Zn^{2+} ions via an excited-state intramolecular proton transfer (ESIPT) mechanism. The sensor demonstrated strong selectivity even in the presence of competing metal ions, with a limit of detection (LoD) of 5.85 ppm. Furthermore, real-water analysis validated its efficient zinc-sensing performance, establishing NapSB as a promising, highly selective, and competitive fluorescent probe for Zn^{2+} detection.

References

1. Peng, H.; Shen, K.; Mao, S.; Shi, X.; Xu, Y.; Aderinto, S. O.; Wu, H., *J. Fluoresc.*, **2017**, *27*, 1191-1200.
2. Tudor, R.; Zalewski, P. D.; Ratnaike, R. N., *J. Nutr health aging*, **2005**, 9, 45-51.
3. Herga, S.; Berrin, J. G.; Perrier, J.; Puigserver, A.; Giardina, T., *FEBS letters*, **2006**, *580*, 5899-5904.

PP 31

Fabrication and Characterization of Iron Porphyrin Nanoparticles for Biomedical Applications

Anaswara Biju M[a], Arun U[b], **Sreeja R**[a,*]

[a]*Department of Physics, Mar Ivanios College (Autonomous), Nalanchira, Thiruvananthapuram, Kerala, 695015, India*

[b]*Department of Biochemistry, Government College, Kariavattom, Thiruvananthapuram*

**sreeja.r@mic.ac.in*

Keywords: Fe (III) porphyrin nanoparticles, MTT assay, Anti-cancer studies

The development of safe and effective nanotheranostics for biomedical applications have drawn increased interest from researchers recently. Herein, we describe the synthesis of Fe (III) porphyrin (TCPP) coordination nanoparticles via a simple co-precipitation method. Characterization techniques including XRD, FTIR, UV Vis and Raman analysis were used to evaluate the physico-chemical properties of the synthesized nanoparticles. The size and structure were evaluated through TEM and SAED examinations. The cytocompatibility of the Fe (III) porphyrin nanoparticles in normal mouse fibroblast L929 cells has been confirmed through the MTT assay. The efficacy of the nanoparticles against melanoma skin tumour was also studied which gives insights into their anticancer activity.

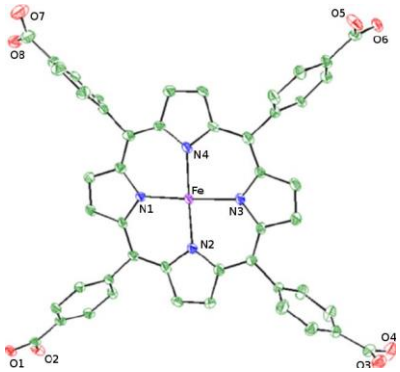


Figure 1 Structure of Fe (III) porphyrin

References

1. Li, S.; Guo, Y.; Liu, L.; Wang, J.; Zhang, L.; Shi, W.; Liu, J., *Catalysts*, **2023**, *13*, 732.
2. Fidalgo-Marijuan, A.; Barandika, G.; Bazán, B.; Urtiaga, M. K.; Arriortua, M. I., *Polyhedron*, **2011**, *30*, 2711-2716.
3. Wang, B.; Dai, Y.; Kong, Y.; Du, W.; Ni, H., Zhao, H.; Fan, Q., *ACS Appl. Mater. Interfaces*, **2020**, *12*, 53634-53645.

PP 32

Imine-Functionalized Chitosan Biosorbent as a pH-Tunable Platform for Efficient Dye Adsorption

Vismaya Joseph[a], Abraham Joseph[a,*]
[a]*Department of Chemistry, University of Calicut, Thenhipalam, Malappuram, India*
**abrahamjoseph@uoc.ac.in*

Keywords: Chitosan, Adsorption, Dye removal, pH

Chitosan is a biopolymer rich in amino and hydroxyl groups, making it a promising candidate for developing biosorbents capable of effectively removing dyes from wastewater. However, unmodified chitosan exhibits several limitations, which can be addressed through chemical modifications and the incorporation of nanoparticles[1,2]. To enhance its structural stability and surface functionality, chitosan was chemically modified via imine functionalization with 3,4-dihydroxybenzaldehyde and crosslinking with glutaraldehyde. The resulting chitosan-based crosslinked gel (ChDBAG) was characterized and compared with bare chitosan without imine functionalization (ChG) using various analytical techniques. The dye removal efficiency of the hydrogel was evaluated across different pH ranges with optimized adsorbent dosage, and dye concentration for both cationic and anionic dyes.

References

1. Crini, G. *et al*. *Environ. Chem. Lett.*, **2019**, *17*,1645-1666.
2. Jawad, A.H.; Mubarak, N.S.A.; Abdulhameed, A. S., *Int. J. Biol. Macromol.*, **2020,** *142*,732-741.

PP 33

One-Step Polymerization of Polyvinyl Alcohol/Cashew Gum/Polypyrrole/Copper Oxide Nanocomposites for High-Performance Flexible Films in Optoelectronics

Ayisha J. Kalladi[a], Jayalakshmi K.[a], Mannammal T. Ramesan[a,*]

[a]*Centre for Polymer Science and Technology, Department of Chemistry, University of Calicut, Calicut University P.O., Malappuram,Kerala, India*

[*]*mtramesan@uoc.ac.in*

Keywords: Cashew gum, copper oxide, Electrical properties, Polyvinyl alcohol, Thermal stability.

A ternary blend nanocomposite composed of polyvinyl alcohol/cashew gum/polypyrrole (PVA/CG/PPy) with varying contents of copper oxide (CuO) nanoparticles was synthesized via an in situ polymerization method, using water as an eco-friendly solvent. Fourier-transform infrared spectroscopy (FTIR), UV–visible spectroscopy, field emission scanning electron microscopy (FE-SEM), x-ray diffraction (XRD), thermogravimetric analysis (TGA), and differential scanning calorimetry (DSC) were used to characterize the ternary blend nanocomposites. FTIR and UV–visible spectra demonstrated strong intermolecular interactions between the functional groups of the PVA/CG/PPy blend and the CuO nanoparticles. XRD patterns revealed that the CuO nanofillers were arranged in a structured manner within the ternary blend matrix. FE-SEM confirmed the uniform dispersion and structured arrangement of CuO nanofillers at a concentration of 3 wt% within the blend matrix. TGA and DSC results showed that the addition of CuO nanoparticles to the PVA/CG/PPy blend improved both the thermal stability and glass transition temperature of the blend matrix. Electrical properties improved with CuO content up to 3 wt%, resulting in enhanced conductivity, an increased dielectric constant, and reduced activation energy. The highest tensile strength, 13.76 MPa, was also observed at this concentration. However, properties declined beyond 3 wt% due to agglomeration, making 3 wt% the ideal concentration for maximum performance. This study highlights the potential of PVA/CG/PPy/CuO nanocomposites for applications requiring improved electrical properties and thermal stability, particularly in flexible electronics and energy storage devices.

References

1. Teles, F.; Antunes, F., *J. Vinyl Addit Technol.*, **2023**, *29*, 120-129.
2. Khlyustova, A.; Evdokimova, A.; Shibaeva, V.; Sirotkin, N., *J. Vinyl Addit. Technol.*, **2024**, *30*, 580-595.

PP 34

Development of an Efficient Green Method (Microwave Assisted) for the Synthesis of Novel 7- Substituted Benzofuran Carbamate Derivatives: *In Silico* and *In Vitro* Approach

M Surendra[a], B Subba Rao[b], P Sanjeeva[b] and P Venkata Ramana[a,*]
[a]Department of Chemistry- Sri Krishnadevaraya University, Ananthapuramu, A.P.
[*]*mylarisurendrasku@gmail.com*

Key words: Microwave assisted (MA), In silico, Molecular docking, ADMET analysis, In vitro, Biological efficacy, Greener synthetic technique, Drug discovery process.

A novel, efficient, and green microwave-assisted (MW) method was developed for the rapid synthesis of a library of 7-substituted benzofuran carbamate derivatives. This protocol minimizes reaction time and solvent usage, offering an environmentally sustainable route to this biologically relevant scaffold.

The synthesized compounds were investigated using an integrated computational and experimental approach. In silico molecular docking and ADMET analysis were performed for initial screening and prediction of drug-like properties. Subsequently, in vitro assays confirmed the biological efficacy of the promising candidates. This combined methodology successfully identified potent and drug-like 7-substituted benzofuran carbamate derivatives, validating both the greener synthetic technique and the streamlined drug discovery process.

References

1. Budhwani, S. N.; Sharma, S.; Kalyane, N., *Asian J. Pharm. Clin. Res.* **2017**, *10*, 377.
2. Kim, S.H.; Pak, H.S.; Lee, M.S.; Cho, Y.J.; Kim, Y.S.; Hwang, J.T.; Sung, M.J.; Kim, M.S.; Kwon, D.Y.; *Biochem. Biophy*. Res. Co, **2008**, *372* 108e113.

PP 35

Effect of Bryophyllum Pinnatum and Tridax Procumbens on Kidney Stone

Nikita Sanjay Kale[a], Nupur M. Jalewar[a], Anusaya S. Chavan[a,*]
[a]*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Maharashtra, India*
**aschavan.chemistry@bamu.ac.in*

Keywords: Bryophyllum pinnatum, Tridax procumbens, Calcium oxalate, Kidney stone, Inhibitory activity.

Kidney stones are a common and painful urological condition, prompting interest in plant-based treatments with fewer side effects. This study evaluates the antiurolithiatic effects of *Bryophyllum pinnatum*[1,2] and *Tridax procumbens*[3], both of which are traditionally used for renal ailments. The effects of the leaf extracts were examined on both synthetic calcium oxalate stones and original kidney stones. The combination of both extracts exhibited greater dissolution and inhibitory activity compared to the individual extracts. These findings support their potential use in developing effective, natural therapies for kidney stone prevention and treatment.

References

1. Yadav, M.; Gulkari, V.; Wanjar, M., *Anc. Sci. Life.*, **2016**, *36*, 90-97.
2. Mety, S.; Channabasava, Kamble, A., *Ann. Clin. Med. Res.*,**2022,** *3*, 1059.
3. Satishchandra, A.; Alagarsamy, V.; Radhika, V.; Ravi Kumar, V.; Narendhar, B.; Bose, P. S. C. *Pharmacogn. Res*., **2023**, *15*, 667-670.

PP 36

Design, Synthesis, and Characterisation of Novel Benzimidazole Derivatives

Nupur M. Jalewar[a], Anusaya S. Chavan[a,*]

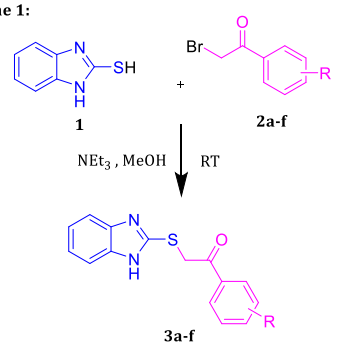
[a]*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Maharashtra, India*

**aschavan.chemistry@bamu.ac.in*

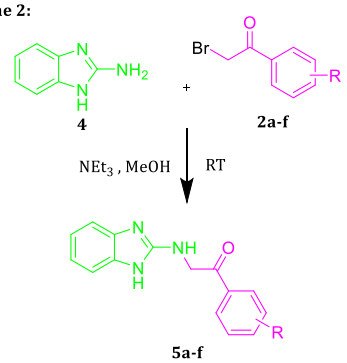
Keywords: 2-Mercaptobenzimidazole, 2-Aminobenzimidazole, Medicinal chemistry, Bioactive scaffolds, Pharmacological relevance.

Benzimidazole derivatives are well-recognised in medicinal chemistry due to their broad spectrum of pharmacological properties, including antimicrobial, anticancer, anti-inflammatory, and antioxidant activities. In this work, a new series of 2-mercapto-benzimidazole (Scheme 1) **3a-f** and 2-amino-benzimidazole (Scheme 2) **5a-f** derivatives was designed, synthesised, and characterised. The synthesis was achieved via efficient protocols under mild conditions, yielding good product conversion. [1,2,3] The study highlights the potential of benzimidazole-based scaffolds as versatile frameworks for developing novel bioactive agents. Further biological evaluation of the synthesised compounds is planned to explore their pharmacological relevance. Other details will be debated during the presentation.

Scheme 1:



Scheme 2:



References

1. Hussain, R.; Ullah, H.; Rahim, F.; Sarfraz, M.; Taha, M.; Iqbal, R.; Rehman, W.; Khan, S.; Shah, S.A.A.; Hyder, S.; Alhomrani, M.; Alamri, S.A.; Abdulaziz, O.; Abdelaziz, M., *Molecules*, **2022**, *27*, 6087.
2. Ullah, H.; Khan, S.; Rahim, F.; Taha, M.; Iqbal, R.; Sarfraz, M.; Shah, S.A.A., Sajid, M.; Awad, M.; Omran, A.; Albalawi, M.; Abdelaziz, M.; Areefy, A.; Jafri, I., *Molecules*, **2022,** *27*, 6921.
3. Hussain, R.; Rahim, F.; Ullah, H.; Khan, S.; Sarfraz, M.; Iqbal, R.; Suleman, F.; Al-Sadoon M. K., *Molecules*, **2023**, *28*, 7015.

PP 37

Ru-Catalyzed Domino C-4-Alkylation and Hydroxylation of Pyrazolones using Alcohols *via* Borrowing Hydrogen Catalysis

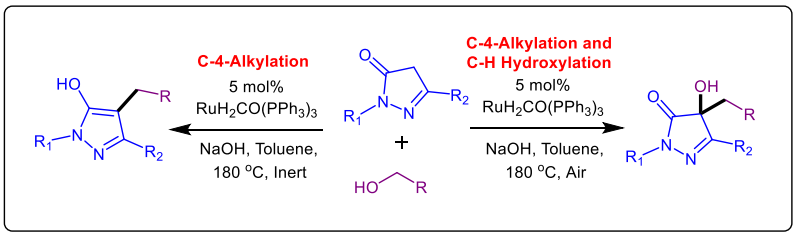
Pramod M. Jadhav[a], Akash B. Jamdade[a], Boopathy Gnanaprakasam[a,*]

[a]*Department of Chemistry, Indian Institute of Science Education and Research, Dr. Homi Bhabha Road, Pune-411008, India.*

**gnanaprakasam@iiserpune.ac.in*

Keywords: Domino Reaction, Ru-Catalyst, Borrowing Alkylation, C-H Hydroxylation, Pyrazolones.

Pyrazolone is a unique and significant five-membered nitrogen-containing heterocycle and have found many applications as a powerful synthons in organic synthesis. It is also prevalent structural motif in many bioactive alkaloids and drugs that function as antipyretic, analgesic, antibacterial, antidiabetic, neuroprotective and anti-infective agents as well as inhibitors for a series of biological enzymes. Due to the structural diversity and reactivity, pyrazolone holds great potential for the development of medicinal and pharmaceutical chemistry, agrochemicals, functional materials and coordination chemistry. Transition metal catalysed borrowing alkylation are well reported in literature by several research groups for the alkylation of active methylene carbon of ketones, amides and esters. Herein, we developed domino approach for the C-4-functionalization of pyrazolones which includes sequential C-4-alkylation and C-H hydroxylation[1] with alcohols to achieve C-4-substituted pyrazolones and pyrazoles *via* borrowing hydrogen catalysis.[2] The method is successfully facilitated in the presence of $RuH_2CO(PPh_3)_3$ catalyst and sodium hydroxide as a base. Notably, this approach has been well validated with the 16 examples of 4-substituted pyrazolones with hydroxylated products and 14 examples of pyrazoles, producing water as the sole environmentally benign byproduct.[3]



References

1. Chaudhari, M. B.; Sutar, Y.; Malpathak, S.; Hazra, A.; Gnanaprakasam, B., *Org. Lett.* **2017**, *19*, 3628-3631.

2. a) Chaudhari, M. B.; Bisht, G. S.; Kumari, P.; Gnanaprakasam, B., *Org. Biomol. Chem.* **2016**, *14*, 9215-9220. b) Jamdade, A. B.; Sutar, D. V.; Bisht, G. S.; Gnanaprakasam, B., *Org. Lett.* **2021**, *23*, 7386–7390.
3. Jadhav, P. M.; Jamdade, A. B.; Gnanaprakasam, B., *Synlett.* **2025**, *Just accepted*.

PP 38

Green Synthesis of Substituted Pyrimido[2,1-B] Quinazolin-7-One *via* Ionic Liquid

Samiksha B. Walse[a], Nupur M. Jalewar[a], Anusaya S. Chavan[a,*]

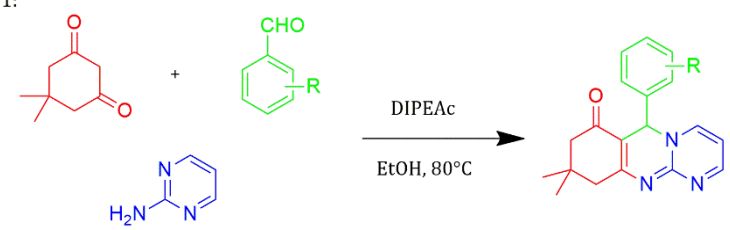
[a]*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Maharashtra, India*

**aschavan.chemistry@bamu.ac.in*

Keywords: Ionic liquid, Multicomponent reaction, pyrimido[2,1-b]quinazolin-7-ones, Fused heterocycles, Bioactive heterocycles.

An efficient and environmentally benign synthesis of substituted pyrimido[2,1-b]quinazolin-7-ones has been developed via a one-pot, Multicomponent reaction of aromatic aldehydes, dimedone, and 2-aminopyrimidine in the presence of the ionic liquid DIPEAc (diisopropylethylammonium acetate) (Scheme 1).[1,2] The reaction proceeds under reflux conditions, affording the target fused heterocycles in good yield. DIPEAc acts as a promoter, offering a recyclable and eco-friendly medium.[3] The methodology aligns with green chemistry principles and provides a practical approach to bioactive heterocycles. Structures of the synthesised compounds are planned to be characterised by using spectral techniques. Other details will be debated during the presentation.

Scheme 1:



References

1. Arora, D.; Arora, S.; Kumar, S.; Kishore, D; Dwivedi, J, *J.Chem.Sci*., **2021**, *133*, 129
2. Shirini, F; Seddighi, M; Jolodar, O, *J. Iran. Chem. Soc.*, **2016,** *13*, 2013–2018.
3. Bhosale, A.; Falke, G.; Bondle, A.; Sarkate, R.; Azad; Burra, P, *Polycycl. Aromat. Compd.* **2023**, *43*, 7912-7929.

PP 39

Comparative Estimation of Vitamin C in Different Fresh Fruits

Sarita A. Shejul[a], Nupur M. Jalewar[a], Anusaya S. Chavan[a,*]
[a]*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Maharashtra, India*
**aschavan.chemistry@bamu.ac.in*

Keywords: Vitamin C, Ascorbic acid, Iodometric titration, Spectrophotometric method, Antioxidant.

This study investigates the vitamin C (ascorbic acid) content in various fruit samples using both iodometric titration[1] and spectrophotometric methods[2]. Fruits such as oranges, lemons, and amla were selected based on their common consumption and known vitamin C richness. The iodometric method involved the reduction of iodine to iodide by ascorbic acid, while the spectrophotometric method provided precise absorbance-based quantification.

A comparative analysis of the two techniques revealed close correlation and confirmed the reliability of both approaches. The isolated vitamin C was further evaluated for its potential applications, such as pharmaceutical formulations, food preservation, and cosmetic products, due to its antioxidant properties.[3,4] These findings highlight variations in vitamin C content among fruits and emphasise the nutritional significance and industrial relevance of this essential nutrient.

References

1. Raman, S.; Sehrawat, A.; Upadhyay, R.; Singh, S.; Verma, A.; Aarushi, Jain, S.; Kanika, Raizada, P. ; Siddhu, A.; Aggarwal, A., *Int. J. Curr. Microbiol. App. Sci*, **2023**, *12*, 56-66.
2. Afnani, F.; Yanti, J. H.; Pratiwi, W. S. W., *Jurnal Kimia Riset*, **2023**, *8*, 116 – 123.
3. Susa, F.; Pisano, R., *Processes*, **2023**, *11*, 3167.
4. Ge, M.; O'Reilly, A.; Baillie, N.; Twentyman, G.; Sturt, J.; Fitzpatrick, M., Taylor, T., *nzfp*, **2008,** *35*, 312-318.

PP 40

Greener Protocol for the Synthesis of Pyrido[2,3-d]Pyrimidine-2,2(1h,3h)-Dione using Ionic Liquid

Siddhi P. Molwane[a], Nupur M. Jalewar[a], Anusaya S. Chavhan[a,*]

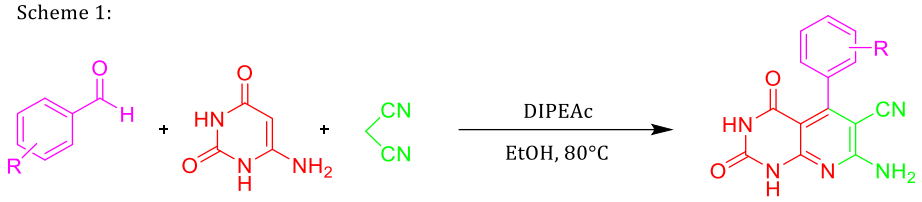
[a]*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Maharashtra, India*

[*]*aschavhan.chemistry@bamu.ac.in*

Keywords: Ionic liquid, Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, Green strategy, Multicomponent reaction, Thermal stability.

Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione is a bioactive heterocycle with diverse pharmacological and synthetic applications. Traditional synthesis involves volatile solvents and harsh conditions, posing environmental benign. This study introduced a greener protocol for the synthesis of pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione derivatives via the multicomponent reaction of 2-amino uracil, substituted aldehydes, and malononitrile using ionic liquid, DIPEAc (diisopropylethylammonium acetate) (Scheme 1) as an alternative medium, leveraging their non-volatility, recyclability, and thermal stability.[1] The method resulted in shorter reaction times, higher yields, and reduced waste. Structures of the synthesised compounds are planned to be characterised by using spectral techniques. Overall, this approach highlights ionic liquids as an effective green strategy for synthesising pyrido[2,3-d]pyrimidine derivatives.[2,3] Other details will be debated during the presentation.

Scheme 1:



References

1. Bhosale, M.; Falke, A.; Bondle, G.; Sarkate, A.; Azad, R.; Burra, P., *Polycycl. Aromat. Compd.* **2023**, *43*, 7912-7929.
2. Nezhadramezan-Ghasemabadi, H.; Mazloumi, M.; Azimi, S.; Shirini, F., *J. Mol. Struct.*, **2023,** *1274*, 134435.
3. Singh, S.; Saquib, M.; Singh, M..; Tiwari, J.; Tufail, F.; Singh, J.; Singh, J., *New J. Chem.*, **2016**, *40*, 63-67.

PP 41

Nonlinear Optical Modulation in Phenyl-Urea Frameworks: A DFT Perspective

Gopika Krishnan G.S.[a], K. Muraleedharan[*]
[a]*Department of Chemistry, University of Calicut, Malappuram 673635, India*
[*]*kmuralika@gmail.com*

Keywords: Phenyl Urea, (hyper)polarizabilities, EOPE, SHG, TDM

The present study investigates the nonlinear optical (NLO) responses of phenyl-urea-based molecules. The optimized geometries of (4-nitrophenyl) urea (PU1), 1-methyl-3-(4-nitrophenyl) urea (PU2), and 1,1-dimethyl-3-(4-nitrophenyl) urea (PU3) were obtained using the M06-2X/6-311++G(d,p) level of theory. The NLO responses were evaluated through static and dynamic hyperpolarizability analyses, supported by dipole moment, polarizability, global reactivity parameters, HOMO–LUMO energy gap, molecular electrostatic potential (MEP) mapping, and β values.[1] Compared to standard NLO materials such as urea and p-nitroaniline, all the designed phenyl-urea derivatives exhibit enhanced NLO activity, with PU3 demonstrating the highest response.[2] The superior NLO behaviour of PU3 is attributed to its smaller HOMO–LUMO gap and stronger intramolecular charge transfer (ICT) characteristics. Furthermore, the dynamic NLO properties, including second-harmonic generation (SHG) and electro-optic Pockels effect (EOPE), indicate the strong potential of these phenyl-urea derivatives as efficient quadratic NLO materials.

References

1. Ahsin, A.; Ayub, K., *J. Nanostruct. Chem.,* **2022***, 12*, 529-545.
2. Bağlan, M.; Gören, K.; Yıldıko, Ü., *Int. J. Chem. Technol.,* **2023***, 7*, 38-47.

PP 42

Molecular Mechanism - Novel Binding Site and Electron Transfer Mechanism of Endothelial Nitric Oxide Synthase Activation by Calreticulin Mediated Transacetylation of Indolyl Fluorochalcones

Rashika G.[a], **Durga M.**[a], Radhika Narayanan Nair[a], Susmita De[a,*]
[a]*Department of Chemistry, University of Calicut, Malappuram - 673635, Kerala, India*
[*]*susmita@uoc.ac.in*

Keywords: Indolyl fluorochalcone, Calreticulin transacetylase, Nitric oxide synthase

Nitric oxide (NO) is a critical signaling molecule in cardiovascular physiology, and its production is regulated by nitric oxide synthase (NOS).[1] The post translational modifications such as acetylation and phosphorylation on amino acids of NOS have shown to modulate the catalytic activity of NOS.[2] In vitro, coupling between calreticulin transacetylase and deacetylation of indolyl fluorochalcone significantly activate endothelial nitric oxide synthase (eNOS), leading to enhanced NO production and anti-platelet effects. However, the mechanism of this activation is unknown.[3] Through molecular docking, molecular dynamics (MD) simulations, and binding energy calculations, we explored the protein–protein interaction between calreticulin transacetylase and eNOS as well as interaction between calreticulin transacetylase and indolyl fluorochalcone, and how these interactions cause conformational changes in eNOS that enhance its activity and increase nitric oxide production [Figure 1]. We identified the binding site of indolyl fluorochalcone on calreticulin and the lysine residues of eNOS, whose acetylation activates eNOS and subsequently enhances nitric oxide production.

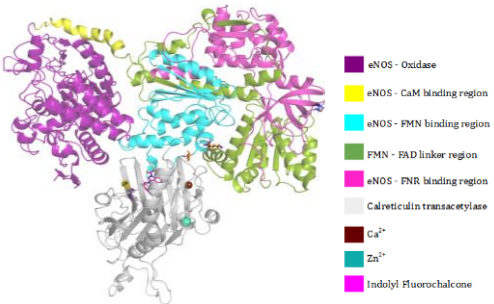


Figure 1. Structure of eNOS and Calreticulin transacetylase bearing Indolyl fluorochalcone

References

1. Underbakke, E. S.; Surmeli, N. B.; Smith, B. C.; Wynia-Smith, S. L.; Marletta, M. A., *Comprehensive Inorganic Chemistry II*, **2013** (2nd Edn)

2. Jung, S. B.; Kim, C. S.; Naqvi,A.; Yamamori, T.; Mattagajasingh, I.; Hoffman, T. A.; Cole, M. P.; Kumar, A.; DeRicco, J. S.; Jeon, B. H.; Irani, K.**,** *Ahajournals*, **2010,** *107*, 877–887.
3. Kumar, A.; Sushama, A.; Manral, S.; Sinha, R.; Joshi, R.; Singh, U.; Rohil, V.; Prasad, A. K.; Parmar, V. S.; Raj, H. G., *Elsevier*, **2012,** *26* **,**9-19.

PP 43

Supercritical CO_2 - Assisted coating of Paracetamol and Aspirin: A Novel Approach for Controlled Drug Delivery

Hridya M.P.[a], Raveendran poovathinthodiyil [a,*]

[a]*Supercritical Fluid Facility, Department of Chemistry, University of Calicut, Kerala-673 635, India.*

[*]*raveendran.pr@gmail.com*

Keywords: Supercritical carbon dioxide, Green solvent coating, Active pharmaceutical ingredient, Excipient, Sustained release, Drug delivery

Supercritical carbon dioxide (Sc CO_2)-based drug coating is an advanced technique that utilizes CO_2 above its critical temperature and pressure, where it exhibits both gas-like diffusivity and liquid-like solvating power. This unique property allows Sc CO_2 to act as a green solvent or anti-sovent for coating acive pharmaceutical ingredients(API) with polymers or excipients without using harmful organic solvents[1]. The method enables uniform, controlled, and solvent-free coatings that can improve drug stability, mask taste, and modify release profiles and efficient alternative to conventional coating process[2].

Pelletized Paracetamol and Aspirin were coated with sucrose octaacetate using supercritical carbondioxide as a green processing medium. The method enabled formation of a consistent coating layer and maintained the structural integrity of the drugs. Analytical studies confirmed successful coating and sustained release behaviour of the treated samples compared to the uncoated ones. This highlights the potential of supercritical CO_2 as an eco-friendly approach for developing controlled drug delivery systems.

References

1. Ramachandran, J. P.; Antony, A.; Ramakrishnan, R. M.; Wallen, S. L.; Raveendran, P., *J. CO2 Util.* **2022**, *59*, 101971.
2. Ramachandran, J. P.; Kottammal, A. P.; Antony, A.; Ramakrishnan, R. M.; Wallen, S. L.; Raveendran, P., *J. CO2 Util.* **2021**, *47*, 101472.

PP 44

Effect of Silver Doping on Structural and Photocatalytic Property of Biosynthesized Copper Oxide Nanoparticles

Latha[a], Nagaraja G.K[a,*]
[a]*Department of Chemistry, Mangalore University, Mangalagangothri, Karnataka, India*
[*] *nagarajagk@gmail.com*

Keywords: Biosynthesis, Ag doped CuO, Photocatalysis, Dye degradation

Pure and Silver doped (2 mol%) Copper Oxide nanoparticles were synthesized using aqueous extract of *Cucumis Mederaspatensis L.* fruit. The biosynthesized nanomaterials were characterized by UV-Diffuse Reflectance Spectroscopy (UV-DRS), Fourier transform infrared spectroscopy (FTIR), X-ray diffraction spectroscopy (XRD), Field emission scanning electron microscopy (FESEM) coupled with Energy dispersive X-ray spectroscopy (EDS), Brunauer-Emmett-Teller (BET) and Barret-Joyner-Halenda (BJH) analysis. The average crystallite size observed was 53 nm and 35 nm for pure and Ag doped CuO nanoparticles respectively calculated using XRD analysis. Tauc plot obtained using UV-DRS was used to calculate band gap of the nanoparticles which was observed to be equal to 4.1 eV and 2.8 eV for pure and doped samples respectively. FTIR spectroscopy confirmed the presence of Cu-O bond. The structural morphology was obtained by FESEM images and EDS analysis validates the elemental composition of the pure and Ag-doped CuO nanoparticles. An increase in the BET surface area from 13.5 to 36.8 cm^2/g was observed for doped nanoparticles. The synthesized nanoparticles were tested for their photocatalytic degradation ability against Crystal Violet (cationic dye) and Methyl Red (anionic dye) solutions. The doped CuO nanoparticles exhibited an excellent degradation efficiency of 98.1% and 99.3% against Crystal Violet and Methyl Red respectively under sunlight irradiation. Thus, the newly synthesized nanomaterials proved to be an interesting photocatalyst for the purification of waste water effluent from textile industries.

PP 45

Fluorescent Sensing Platform Based on Nitrogen-Doped Carbon Dots-ZIF-67 Composite for Selective Bovine Serum Albumin Detection in Simulated Body Fluids

Maneesha M[a], Preethi P. C[a,b], Harisankar A[a,c], Sreeja T G[d], Ratheesh Kumar V K[a], Sreevidya Thekku Veedu[e], Resmi Raghunandan [a,*]

[a]*Postgraduate and Research Department of Chemistry, Mahatma Gandhi College, University of Kerala, Thiruvananthapuram, 695004, Kerala, India.*

[b]*Department of Science and Humanities, Mar Baselios College of Engineering and Technology, Thiruvananthapuram, 695015, Kerala, India.*

[c]*Department of Basic Science, Bishop Jerome Institute, School of Engineering, Kollam 691001, Kerala, India*

[d]*Department of Chemistry, VeluThampi Memorial Nair Service Society College, Dhanuvachapuram, University of Kerala, Thiruvananthapuram 695503, Kerala, India*

[e]*Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, 22607 Hamburg, Germany*

[*]*resmiraghu@mgcollegetvm.ac.in*

Keywords: Metal-organic framework, Composites, Biomarker, Sensing, Albumin

BSA is an important biomarker as the lower levels in the blood (hypoalbuminemia) are a sign of liver failure and chronic hepatitis, while higher level (hyperalbuminemia) in the blood is accompanied by edema and shock. So, the sensing and quantification of albumin in body fluids are crucial for the wellness of an individual. In this study, ZIF-67 functionalized with nitrogen-doped carbon dots (N-CQDs) is designed for the ultra-sensitive and selective detection of BSA. The N-CQD@ZIF-67(NCZ-67) composite material was synthesized through a facile process, leveraging the unique photoluminescent properties of nitrogen-doped carbon dots and the robust structural framework of ZIF-67. The synthesized composite is characterized using FT-IR, UV-visible spectroscopy, and photoluminescence spectroscopy. It serves as a highly efficient 'turn-on' sensor for detecting bovine serum albumin (BSA) with a limit of detection (LOD) of 0.2129 μM. The sensing mechanism operates via Förster Resonance Energy Transfer (FRET). The applicability was further confirmed by detection in simulated body fluids. The study underscores the potential of N-CQD@ZIF-67 in developing next-generation biosensors, particularly for the early detection and monitoring of liver and kidney-related disorders.

References

1. He, Y.; Yu, Z.; He, J.; Zhang, H.; Liu, Y.; Lei, B., *Sens. Actuators, B Chem.,* **2018**, *262,* 228–235.

2. Ksenofontov, A.A.; Bocharov, P.S.; Ksenofontova, K. V.; Antina, E. V., *J. Mol. Liq.* **2022**, *345,* 117031.
3. Mati, A.; Senoussi-Ghezali, C.; Si Ahmed Zennia, S.; Almi-Sebbane, D.; El-Hatmi, H.; Girardet, J.M., *Int. Dairy J.* **2017**, 73, 25–37.

PP 46

Promotive Effect of Buffer-Ion Cofactors on Two-Electron Water Oxidation Catalyzed by Vanadium Porphyrins

Muhammad Ameen[a], Arifa Kaniyantavida[a], Jayachandran Kaippully[a], Haritha Anamangattupurakkal[a], Aparna chencharodi[a], Sebastian Nybin Remello[b], Hiroshi Tachibana[c], Haruo Inoue[c], Fazalurahman Kuttassery[a,*]

[a]*Department of Chemistry, University of Calicut, Malappuram 673635, Kerala, India.*

[b]*Department of Applied Chemistry, Cochin University of Science and Technology, Kerala, India.*

[c]*Department of Applied Chemistry, Tokyo Metropolitan University, Japan.*

[*]*kfazalurahman@uoc.ac.in*

Keywords: Artificial photosynthesis, Vanadium porphyrins, Hydrogen Peroxide.

Artificial photosynthesis represents a biomimetic approach to converting sunlight into chemical fuels, offering a sustainable route for energy production. However, the conventional four-electron oxygen evolution reaction (OER) catalyzed by molecular catalysts is intrinsically sluggish due to the requirement to accumulate multiple redox equivalents at the reaction center [1–2]. We have previously shown that the cationic vanadium porphyrin catalyst VOTMPyP can promote an alternative two-electron pathway, producing hydrogen peroxide as the primary product at pH 12.5 with an overall Faradaic efficiency of 93.5%. The current challenge is to enhance the selectivity toward two-electron product (H_2O_2) and to drive the catalytic cycle under moderate pH conditions. To address this, we investigated the effects of two buffer systems—carbonate and borate—on the catalytic activity of VOTMPyP, revealing improved electrochemical performance. Reaction kinetics in these buffers were analyzed using a modified Randles–Sevcik method. The catalytic turnover frequency (TOF) was $3.55 \times 10^4\ s^{-1}$ in carbonate buffer (pH 9.8) and $1.10 \times 10^4\ s^{-1}$ in borate buffer (pH 8.3). The observed enhancement in TOF and the improved selectivity for H_2O_2 relative to non-buffered conditions highlight the potential applicability of this system in artificial photosynthetic devices.

References

1. Kuttassery, F.; Mathew, S.; Remello, S. N.; Thomas, A.; Sano, K.; Ohsaki, Y.; Nabetani, Y.; Tachibana, H.; Inoue, H., *Coord. Chem. R*ev., **2018**, ***377***, 64-72.
2. Kuttassery, F.; Ohsaki, Y.; Thomas, A.; Kamata, R.; Ebato, Y., Kumagai, H.; Nakazato, R.; Sebastian, A.; Mathew, S.; Tachibana, H.; Ishitani, O.; Inoue, H., *Angew. Chem. Int. Ed.*, **2023,** *62*, e202308956.

PP 47

Study of Structural, Morphological and Magnetic Properties of Copper Ferrite and Nickel Ferrite Nanoparticles

K Ahalya[a], **Naveena-E**[b,*]
[a]*The Zamorins Guruvayurappan College, Calicut*
[b]*Malabar Christian College, Calicut*
**naveenaedakkoth@gmail.com*

Keywords: Spinel ferrites, Magnetic studies, Nano powders, Morphology of iron oxides

Ferrite nanoparticles have attracted significant attention in recent years because of their unique electrical, magnetic, and structural properties, which are distinct from their bulk counterparts. Among them, copper ferrite ($CuFe_2O_4$) and nickel ferrite ($NiFe_2O_4$) are of particular importance due to their stable spinel structure, tunable particle size, and wide range of technological applications. Their nanoscale nature enables enhanced surface-to-volume ratio, improved crystallinity, and altered magnetic ordering, making them promising candidates for advanced electronic and magnetic devices.

In the present study, $CuFe_2O_4$ and $NiFe_2O_4$ nanoparticles were synthesized using a low-cost and facile co-precipitation method, chosen for its simplicity, reproducibility, and ability to control particle growth. The synthesis was carried out at different pH values (8 and 11) and sintering temperatures (300°C and 800°C) to study the influence of reaction conditions on the final structural and physical properties. Optimization of these parameters is expected to directly affect the crystallite size, degree of agglomeration, and overall stability of the nanoparticles.

The prepared samples underwent a series of characterization techniques to confirm formation and evaluate their fundamental properties. X-ray Diffraction (XRD) analysis was performed to identify the crystalline phase, confirm the cubic spinel structure, and calculate the average crystallite size. Scanning Electron Microscopy (SEM) was employed to study the surface morphology and particle distribution, while Energy Dispersive Spectroscopy (EDS) verified the elemental composition and chemical purity of the synthesized ferrites. Furthermore, Vibrating Sample Magnetometer (VSM) measurements were conducted to evaluate magnetic behavior, including saturation magnetization and coercivity, under different synthesis conditions.

By focusing exclusively on synthesis and characterization, this study aims to establish clear correlations between processing parameters (pH and temperature) and the resulting physical properties of copper and nickel ferrite nanoparticles.

References

1. Ihab, A.; Latif, A., *J. Phys.*, **2012**, *1*, 50–53.
2. Shedam, R. M.; Kashid, P. P.; Mathad, S. N., *Phys. Chem. Solid State*, **2022**, *22*, 626-640.
3. Sudhakaran, S. & Madhavan, V. E. *Langmuir* **2025**, *41*,15841–15848.

PP 48

Single Crystalline Cobalt Molybdenum Oxide Synthesized at n-Butanol/Water Interface for Non-Enzymatic Electrochemical Detection of Epinephrine

Pranav Mecheri[a], Mini Mol Menamparambath[a,*]

[a]*Department of Chemistry, National Institute of Technology Calicut, Calicut-673601 Kerala, India.*

[*]*minimol@nitc.ac.in*

Keywords: Liquid/liquid interface, Electrochemical sensor, Epinephrine.

An interface is an efficient soft-template for the controlled synthesis of nanostructures with distinct morphologies. It can offer a unique quasi-2D interface with higher surface energy for precursor assembly to start the nucleation process, which then spurs intermediate growth to build the desired final structure. The air/liquid, air/solid, liquid/liquid, and liquid/solid interfaces are frequently used for the fabrication of various innovative materials. Among these, synthesis employing a liquid/liquid interface offers a scalable way to create hybrid materials. Here we synthesized cobalt molybdenum oxide hydrate (CMO) using an n-butanol/water interface. XRD, Raman, and FTIR analyses confirmed the formation of monoclinic CMO with the highest crystallinity. The morphology of the synthesized product was examined using SEM and TEM, which revealed well-defined nanorod-like structures. High-resolution TEM and SAED patterns further confirmed the single-crystalline nature of the synthesized compounds. The material was then employed for the electrochemical detection of the neurotransmitter epinephrine, exhibiting excellent sensitivity, selectivity, and repeatability, with a low limit of detection (LOD) of 2.14 nM.

References

1. R. R. Poolakkandy; S. K. Chondath; N. Puthiyottil; D. Davis; M.M. Menamparambath, *Langmuir*, **2020**, *36*, 872
2. S. K. Chondath; M.M. Menamparambath, *Faraday Discuss*, **2023**, *247*, 227
3. Mecheri. P; Hareesh. P; Menamparambath. M. M, *Langmuir*, **2025**, *41*, 9422-9433.
4. Rehman. S. U.; Musuvadhi Babulal. S.; Wu. H. F, *ACS Appl. Nano. Mater.* ,**2024**, *7*, 25004-25013

PP 49

Ecofriendly Hydrothermal Route for the Synthesis of Graphene Quantum Dots with Photocatalytic Activity

Ranjith V[a], Sanjay Annarao[a,*], Adithi N[b]
[a]*Department of PG Chemistry, University College Hampanakatta, Mangalore, Karnataka, India*
[b]*Department of Chemistry,Mangalore University, Mangalagangothri, Mangalore, Karnataka, India*
[*] *Sanjaymulge@gmail.com*

Keywords: Quantum dots, Phyto-extract, Hydrothermal method, Surface morphology, Dye degradation.

In this study, graphene quantum dots (GQDs) were synthesized via a green hydrothermal method using natural carbon source *Aristolochia indica*. The eco-friendly synthesis route eliminates the need for toxic chemicals and provides a sustainable approach to nanomaterial preparation. The structural and optical properties of the GQDs were characterized using UV–Visible spectroscopy, photoluminescence, and FTIR analyses. The synthesized GQDs exhibited strong absorption in the visible region, indicating their suitability for photocatalytic applications. The photocatalytic efficiency of the GQDs was evaluated by the degradation of a model dye pollutant under natural sunlight exposure. The results revealed that the GQDs showed significant degradation activity, attributed to their high surface area, tunable band gap, and efficient charge separation. This work demonstrates that green-synthesized GQDs can serve as an effective, sustainable photocatalyst for wastewater treatment and environmental remediation.

References

1. Jo, G.; Choe, M.; Lee, S.; Park, W. *Nanotechnology*, **2012**, *23*, 112001.
2. Kumar, S.; Ojha, A.K.; Patrice, D.; Yadav, B.S.; Materny, A. *Phys. Chem. Chem. Phys.* **2016**, *18*, 11157–11167.

PP 50

N-doped Red Emissive Carbon Nanodots for Emission Shift Mediated Moisture Sensing and Bioimaging Applications

Ritu G.[a] , Nidhisha V[a], Renuka Neeroli Kizhakayil[a,*]

[a]*Materials Engineering Lab, Department of Chemistry, University of Calicut, Kerala-673635, India.*

[*]*renuka@uoc.ac.in*

Keywords: Red emissive carbon nanodots, Emission shift, Moisture analysis, Cell imaging , Solvatochromism.

Traditional fluorophores, such as organic dyes and rare earth phosphors, offer intense luminescence. However, they suffer from drawbacks including fixed emission wavelengths, large particle size, low sensitivity, photobleaching, and poor chemical stability. In contrast, carbon nanodots (CNDs), luminescent carbon nanoparticles exhibit tunable emission, ultrasmall size (less than 10 nm), excellent biocompatibility, high water solubility, and minimal toxicity, making them promising candidates for advanced imaging and sensing applications[1].

Here, we report fluorescence-based moisture sensing, and cell-imaging applications of p-phenylenediamine-derived carbon nanodots (PD-CNDs) synthesized via hydrothermal method. The PD-CNDs exhibit solvatochromism, displaying distinct fluorescence colors in different solvents[2]. The solvatochromic behaviour of PD-CDNDs enables precise prediction of solvent pair compositions, based on which accurate moisture detection in acetone, an essential solvent across industries, was realised with over 99% accuracy. Additionally, CNDs serve as a sustainable alternative for cell imaging, owing to its attractive photostability and biocompatibility. Notably, solvatochromic PD-CNDs stand out among other standard CNDs, for their bright emission in organic fixatives, enabling consistent imaging results.

References

1. Gopal, R.; Nidhisha, V.; Amrutha, T.; Aswathi, A.; Midhila, P.; Kurunthatil Kuttiat, T.; Das, S.; Kizhakayil, R. N., *ACS App. Opt. Mat.*, **2023**, *1.3*, 701-714.
2. Nidhisha, V.; Gopal, R.; Anjali, C.; Amrutha, T. P.; Arunima, K. K.; Praveen, V. K.; Kizhakayil, R. N. *Nanoscale Adv.*, **2024**, *6*, 1535-1547.

PP 51

A Facile and Green Method for the Bulk Preparation of Graphene from Graphite using Sc-CO_2

Rubeena T.P[a], Poovathinthodiyil Raveendran[a,*]

[a]*Department of Chemistry, University of Calicut, Kerala-673635, India*

**raveendran.pr@gmail.com*

Keywords: Graphite exfoliation, Supercritical CO_2, Few layer graphene

Graphene, building block of other forms of carbon atoms such as graphite, carbon nanotubes and fullerenes are a remarkable material with a hexagonal, two-dimensional network of sp^2 -hybridized carbon atoms. Since its discovery in 2004, graphene has attracted a lot of attention because of its exceptional properties, which include high mechanical strength, high thermal conductivity, high electrical conductivity, high optical transparency, and a large surface area. These attributes make graphene a very versatile material with a wide range of potential applications in numerous industries. Numerous graphene layers make up graphite, which is kept together by weak, non-directional van der Waals attraction between neighbouring layers that is 0.34 nm long[1].

The present invention outlines a facile, environmentally benign, and solvent-free approach for the bulk production of graphene from graphite utilizing supercritical carbon dioxide ($scCO_2$). The method involves the initial ball milling of graphite in the presence of a CO_2-soluble additive AGLU[2], to achieve a homogenous mixture. This mixture is subsequently subjected to $scCO_2$ conditions, wherein the temperature and pressure exceed the critical point of carbon dioxide. Under these conditions, $scCO_2$ effectively infiltrates the interlayer spaces of graphite. Upon rapid depressurization, the expansion of CO_2 generates a normal force perpendicular to the graphene planes, facilitating the exfoliation of graphite into few-layer or single-layer graphene sheets[3,4,5]. Following this process, the CO_2-soluble AGLU is removed, leaving behind high-quality graphene. This method offers a sustainable and scalable route to graphene production, eliminating the need for hazardous solvents or intensive chemical treatments.

References

1. Sawant, S. Y.; Somani, R. S.; Cho, M. H.; Bajaj, H. C., *RSC Adv.* **2015**, *5*, 46589 - 46597.
2. Raveendran, P.; Wallen, S. L., *ACS Symposium Series; American Chemical Society* **2003**; *860*, 270 - 284.
3. Islam, A.; Mukherjee, B.; Pandey, K. K.; Keshri, A. K., *ACS Nano* **2021**, *15*, 1775 - 1784.
4. Chen, Z.; Miao, H.; Wu, J.; Tang, Y.; Yang, W.; Hou, L.; Yang, F.; Tian, X.; Zhang, L.; Li, Y., *Ind. Eng. Chem. Res.* **2017**, *56* , 6939 - 6944.
5. Wang, Y.; Chen, Z.; Wu, Z.; Li, Y.; Yang, W.; Li, Y., *Langmuir* **2018**, *34* , 7797 - 7804.

PP 52

2D Nano Sheets Prepared from Salicylidene-2-Anthrylamine for the Detection of Warfare Agent Simulant Diethyl Chloro Phosphate

Sarika K.[a], Saranya K. P.[a], Dr. Shanthil M.[a,*]

[a]*Dept of Chemistry, Govt Victoria College, Palakkad- affiliated under University of Calicut.*

**shanthilm@gmail.com*

Keywords : 2D Nano sheet, Solid state emission, Warfare agent simulant.

Two-dimensional soft materials have garnered significant attention from the research community due to large surface area/volume ratio, porosity, flexibility and easy functionalization aside from graphene. Their enhanced physical and optical and properties supports applications in catalysis, OLEDs, energy storage, bio imaging, and semiconducting devices. In this work, we synthesized a metal-free two-dimensional sheet-like material, 2ASD, in the nano regime, derived from the Schiff base Salicylidene-2-anthrylamine (2ASD). This compound forms a layered structure in its solid state due to the dimeric existence of the keto isomer of 2ASD[1]. The weak interactions within the structure enable the easy exfoliation of 2ASD into nanosheet-like forms through simple ultrasonication. We successfully exfoliated 2ASD in water using ultrasonication, resulting in a stable dispersion that exhibited the same emission characteristics as the solid form. The resulting 2D films were drop-casted onto FTO/glass substrates and characterized using spectroscopic and microscopic methods. High-Resolution Transmission Electron Microscopy (HRTEM) images of 2ASD revealed 10 to 20 stacked layers, while Atomic Force Microscopy (AFM) measurements confirmed an average thickness of approximately 15 nm. The material coated on glass plates displayed high luminescence and retained the characteristic keto emission, as evidenced by emission studies[2-4].

Diethylchlorophosphate (DCP), a simulant for the lethal nerve agent Sarin, was used to test the sensitivity of the 2D 2ASD coated glass slides[5]. We observed a shift in the emission spectra of the slides when exposed to DCP vapors. Time-dependent fluorescent spectral shifts and quenching were also noted during exposure to DCP vapors in a sealed cuvette. The selectivity and sensitivity of the material were further assessed using other simulants like dimethyl methoxy phosphonate and phosphoric acid. The reaction of the imine linkage with DCP, which leads to phosphorylation, was confirmed through Infrared (IR) analysis.

References

1. Saranya, K. P.; Ismail, T. M.; Kavya, P.; Vishnu, V. G.; Santhi, V.; Vinayakan, R. N.; Shanthil, M.; Sajith, P. K., *New J. Chem.* **2025**, *49*, 5078 - 5086.

2. Zhou, Z.; Xiao, Y.; Tian, J.; Nan, N.; Song, R.; Li, J., *J. Mat. Chem. A.*, **2023**, *11*, 3245 - 3261.
3. Zhu, D.; Verduzco, R., *ACS Appl Mater Interfaces.* **2020**, *12*, 33121 - 33127.
4. Gao, Q.; Li, X.; Ning, G.-H.; Leng, K.; Tian, B.; Liu, C.; Tang, W.; Xu, H.-S.; Loh, K. P., *Chem. Commun.* **2018**, *54*, 2349 - 2352.
5. Sun, C., Xiong, W., Ye, W., Zheng, Y., Duan, R., Che, Y., Zhao, J., *Anal. Chem.* **2018**, *90*, 7131 - 7134.

PP 53

Advancing Perovskite Stability: A Comparative Study of Lead and Mixed Tin-Lead Materials under Humid Environments

Shana Sudhakaran[a], Vinod E. Madhavan[a,*]

[a]*Department Of Materials Science and Engineering National Institute of Technology Calicut, Kerala, India*

[*]*vinodem@nitc.ac.in*

Keywords: Lead -Tin Mixed perovskite, $MAPbI_3$, Solar cell, Stability

This research explores the stability and degradation processes of lead-based $MAPbI_3$ and tin-lead mixed $MAPb_{0.8}Sn_{0.2}I_3$ perovskite thin films when exposed to humid conditions (60% relative humidity) over a span of 28 days. The study tackles two major issues in perovskite solar cell technology: the toxicity linked to lead content and the inherent instability in ambient environments.[1,2] Employing various characterization methods such as X-ray diffraction (XRD), scanning electron microscopy (SEM), and UV-VIS-NIR spectroscopy, this research elucidates significant differences in the degradation behaviours of the two compositions. $MAPbI_3$ exhibited enhanced stability, forming a potentially reversible monohydrate phase, $MAPbI_3.H_2O$ and the evolution of crystallite size is shown in figure 1, whereas $MAPb_{0.8}Sn_{0.2}I_3$ underwent rapid degradation and loss of crystallinity. Morphological analysis indicated that both compositions underwent significant surface changes, transitioning from well-defined grain structures to porous, coarse surfaces over time. Optical characterization indicated that the inclusion of tin caused a red shift in the absorption edge and a decrease in the band gap. The results emphasize the intricate trade-offs between stability, toxicity reduction, and optical properties in perovskite materials. While incorporating tin offers potential for band gap engineering and reduced lead content, it significantly compromises stability encapsulation techniques and further optimization of tin-lead mixed perovskites to achieve a balance between stability and desired electronic properties for effective and durable solar cell applications.

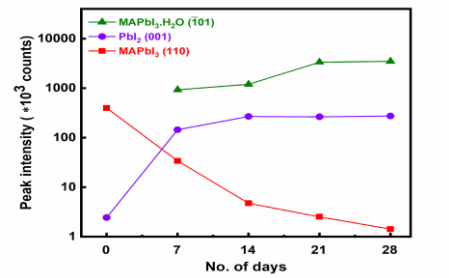


Figure 1: Evolution of X-ray diffraction peak intensity over time caption .[3]

References

1. Singh, R.; Hu, H.; Feeney, T.; Diercks, A.; Laufer, F.; Li, Y.; Duong, T.; Schackmar, F.; Nejand, B. A.; Paetzold, U. W., *ACS Appl. Mater. Interfaces* **2024**, *16*, 27450 - 27462.
2. Zeng, J.; Wang, J.; Wang, J.; Li, J.; Chen, J.; Wei, F.; Zhang, J.; Song, W.; Fan, X., *ACS Nano*. **2024**, *18*, 31390–31400.
3. Sudhakaran, S.; Madhavan, V. E.; *Langmuir* **2025**, *41*,15841–15848.

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Sustainable Preparation of Reduced Graphene Oxide *via Punica Granatum* Extract and its Role in Photocatalytic Dye Degradation

Shivu[a], Sanjay Annarao[a,*], Adithi N[b]

[a]*Department of PG Chemistry, University College Hampanakatta, Mangalore, Karnataka, India*

[b]*Department of Chemistry,Mangalore University, Mangalagangothri, Mangalore, Karnataka, India*

[*] *Sanjaymulge@gmail·com*

Keywords: Hydrothermal method, Chemical properties, Photo oxidizers, Photocatalytic degradation.

Green synthesis of reduced graphene oxide (rGO) has gained momentum over chemical methods due to its environmental compatibility. The present study investigates the effect of reduced graphene oxide (rGO), prepared via green synthesis using plant (phyto) extract *Punica granatum*, on the photocatalytic degradation of organic dyes. The phyto extract acts as a natural reducing and stabilizing agent, replacing hazardous chemicals and promoting an eco-friendly synthesis route. The synthesized rGO was characterized using techniques such as UV–Vis, FTIR, XRD and SEM to confirm reduction, structural formation and surface morphology. The photocatalytic activity of rGO was tested against a selected dye under visible light irradiation. Results revealed that the phyto-synthesized rGO exhibited enhanced photocatalytic efficiency compared to chemically synthesized counterparts, due to its high surface area and improved charge carrier separation. The study demonstrates that green-synthesized rGO can serve as a sustainable and effective photocatalyst for wastewater treatment and environmental remediation.

References

1. Thakur, S.; Karak, N. *Carbon N. Y.* **2012**, *50*, 5331–5339.
2. Zaaba, N.I.; Foo, K.L.; Hashim, U.; Tan, S.J.; Liu, W.W.; Voon, C.H. *Procedia Eng.* **2017**, *184*, 469–477

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Synthesis of rGO from Strychnous Potatorum Phyto-Extract and Study of Photocatalytic Degradation by Hydrothermal Method

Swathi Nayak[a], Sanjay Annarao[a,*], Adithi N[b]

[a]*Department of PG Chemistry, University College Hampanakatta, Mangalore, Karnataka, India*

[b]*Department of Chemistry, Mangalore University, Mangalagangothri, Mangalore, Karnataka, India*

[*]*Sanjaymulge@gmail.com*

Keywords: Reduced graphene oxide, Hummer method, Phyto extract, Physico chemical properties, Photocatalysis.

Industrial chemical pollutants such as methylene blue (MB) dye are released into the water body and potentially cause harm to the human and aquatic biosphere. Therefore, this study aims to synthesize eco-friendly nanocatalysts, i.e., reduced graphene oxide (rGO) for efficient photocatalytic degradation of MB dye. In this study, reduced graphene oxide (rGO) was synthesized using *Strychnous potatorum* extract as a green reducing agent through a hydrothermal method. The natural phytochemicals present in the extract acted as efficient and eco-friendly reducing and stabilizing agents for the conversion of graphene oxide (GO) into rGO, eliminating the need for hazardous chemicals like hydrazine. The synthesized material was characterized using techniques such as UV–Visible spectroscopy, FTIR, and XRD to confirm the successful reduction and structural modification of GO. The photocatalytic activity of the obtained rGO was evaluated through the degradation of a model organic dye under electromagnetic solar radiation. The results revealed that rGO exhibited excellent photocatalytic efficiency due to its high surface area, enhanced charge separation, and strong light absorption capacity. This work demonstrates a sustainable and cost-effective approach for producing reduced graphene oxide using a plant-based extract, promoting green nanotechnology for environmental remediation and dye degradation applications.

References

1. Zaaba, N.I.; Foo, K.L.; Hashim, U.; Tan, S.J.; Liu, W.W.; Voon, C.H., *Procedia Eng.* **2017**, *184*, 469–477.
2. Thakur, S.; Karak, N., *Carbon*, **2012**, *50*, 5331–5339.

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Hydrogenation of Nitroarene using Molybdenum-Nickel based Hydrotalcite Catalyst

Vrinda T. V.[a], Gopika. M.G[a], A. Sakthivel[a,*]

[a]*Inorganic Materials & Heterogeneous Catalysis Laboratory, Department of Chemistry, School of Physical Sciences, Central University of Kerala, Kasaragod – 671320, India.*

**sakthivelcuk@cukerala.ac.in*

Keywords : Hydrotalcite, Nickel, Molybdenum, Sustainable catalysis, Nitroarenes

Fossil fuels and petroleum-derived chemicals have long dominated global energy and industrial sectors. However, their depletion and environmental impact have intensified the search for sustainable catalytic processes. Therefore, the design of efficient, cost-effective catalysts is essential for advancing green chemical transformations.[1] Transition-metal oxides, zeolites, and perovskite-type materials exhibit remarkable catalytic versatility due to their tunable redox and acid–base properties. Layered double hydroxides (LDHs) further advance as potential precursors for future catalysts owing to their distinctive layered architecture and compositional flexibility.[2] The introduction of reactive species as alternatives to noble metal ions, having similar electronic properties and stability, is of great interest. In this regard, metal carbides act as analogues to noble metal species, potentially serving as sustainable alternatives for catalysts used in hydrogenation and hydrotreating of various organic and biomass components.[3]

Incorporation of metal carbides into nickel-based hydrotalcite materials was explored for the hydrogenation of nitroarenes through strong metal–carbide interfacial interactions and uniform active-site dispersion.[4] This work employed Mo-intercalated NiCo and NiFe hydrotalcite precursors subjected to temperature-programmed reduction. The resulting catalysts exhibited highly dispersed and well-integrated alloy–carbide interfaces, which facilitated efficient hydrogen activation and selective reduction of nitro groups. Under optimised reaction conditions, the catalysts achieved near-complete conversion of nitrobenzene with excellent selectivity toward aniline, demonstrating a sustainable and scalable route for fine chemical synthesis.

References

1. Akmach, D., Bathla, S., Tran, C.C., Kaliaguine, S., Mushrif, S., *Catal. Today*, **2023**, *423*, 114285.
2. Neethu, P., Sreenavya, A., Sakthivel, A., *Appl. Catal. A: Gen.*, **2021**, *623*, 118292.
3. Li, Z.; Wang, Y., *Acad. J. Sci. Technol.*, **2023**, *5*, 209–214.
4. Ma, Y., Guan, G., Hao, X., Cao, J., Abudula, A., *Renew. Sustain. Energy Rev.*, **2017**, *75*, 1101–1129.