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Vellore Institute of Technology

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Book of Abstracts

ICMES-2026

International Conference on Organic and Inorganic Materials for Energy and Sustainability

10-12 September

VIT Vellore

India

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(Deemed to be University under section 3 of UGC Act, 1956)

ICMES-2026

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ABOUT VIT

Vellore Institute of Technology (VIT) was founded in 1984 as Vellore Engineering College by the Honorable Chancellor Dr. G. Viswanathan. The institution has grown steadily since its humble beginning. VIT attracts students from all over India and abroad because of its excellence. VIT has emerged as one of India's best institutes and aspires to become a global leader in education. In Engineering and Technology, VIT is ranked 119th in the World and 6th in India (QS World University Rankings by Subject 2026). In Data Science and AI subject areas, VIT is within the top 200 in the world, whereas four subjects (CS, Information Systems, Electrical and Electronics) have been ranked among the top 100 in the world (QS World University Rankings by Subject 2026). It is within the top 2 in India and top 600 in the world (Shanghai ARWU ranking 2025). VIT achieved NAAC Accreditation with A++ grade (3.66 out of 4). VIT is within the top 20 in University, Research and Engineering categories in India (NIRF Ranking, Govt. of India 2025). It secures rank 352nd in the world and 7th in India (QS World University Rankings: Sustainability 2026).

ABOUT THE CONFERENCE

ICMES 2026 will provide an excellent platform to present and discuss cutting-edge research in organic and inorganic materials for energy and sustainability. The conference will feature scientific talks by distinguished international speakers from top 100 QS-ranked universities, along with lectures by eminent faculty from premier Indian institutions such as IISc, IITs, IISERs, and NITs—making it a key highlight of the event. Expert lectures, complemented by interactive sessions with scholars and students, will foster future growth and collaborative opportunities. In addition, participants will present their work through oral and poster sessions, with the best contributions will be recognized through exciting prizes.

ABOUT CHEMISTRY DEPARTMENT

Chemistry department comes under the School of Advanced Sciences (SAS), which was established in the year 1984. Department of Chemistry's vision is to provide quality teaching and research which would make an impact at a global level. The department consists of a total of 77 experienced and energetic faculty. Most of them are experts in their research fields, evident from their publications and research funding. The Department is recognized by DST-FIST to establish sophisticated instrumental facilities. It is also equipped with necessary instruments for research and offers services to other institutions as well. After graduation, students are placed in reputed companies in India and abroad, and they have been securing admissions in India and abroad for their higher education. We offer 2 years MSc and 5 years integrated MSc program in Chemistry. Our MSc program (2 years)

offers specialization in Analytical/Inorganic/Organic/General/Pharmaceutical Chemistry. Our MSc Chemistry program is Accredited by RSC, UK. The subject Chemistry in VIT is ranked within the top 9 in India and top 251-300 in the world as per QS World University Rankings by Subject 2026.

TOPICS OF THE CONFERENCE

- Advanced Functional Materials
- Light-driven Reactions and Materials
- Energy Materials
- Nanomaterials
- MOF & COF
- Synthetic Organic Chemistry
- Total Synthesis
- Drug Design and Medicinal Chemistry
- Organometallics and Catalysis
- Bioinorganic and Bioorganic Chemistry
- Spectroscopy and Instrumentation
- Theoretical and Computational Chemistry
- Green and Sustainable Chemistry
- Environmental Remediation

Dr. G. VISWANATHAN
Founder & Chancellor
Former Member of Parliament
Former Minister, Govt. of Tamil Nadu
President, Education Promotion Society for India, New Delhi

MESSAGE

I am delighted that the Department of Chemistry, School of Advanced Sciences, VIT, Vellore is organizing an **International Conference on "Organic and Inorganic Materials for Energy and Sustainability" (ICMES-2026)** during September 10-12, 2026. The primary purpose of this conference is to provide a common platform for scientists to stimulate and develop their curiosity and creativity in translational research. This meeting is expected to foster scientific interaction among leading researchers from both academia and industry worldwide in the areas of organic and inorganic materials for energy and sustainability.

Advantageously, participants will have the opportunity to establish professional collaborations with universities and researchers across the world, paving the way for the exchange of fresh ideas and innovative discoveries. Such collaborations will ultimately contribute significantly to the nation's continued progress and prosperity in science and technology in the years to come.

We have invited distinguished professors from several countries to this conference to share their expertise, knowledge, and insights with all of us. We have also invited eminent experts from leading national institutions, including IITs, IISERs, CSIR laboratories, Central Universities, and the Department of Atomic Energy (DAE). In addition, participants will have the opportunity to present their research through oral and poster sessions.

I sincerely appreciate the organizers for providing students and researchers with a valuable platform to showcase their research through oral and poster presentations. The dedicated team of faculty members from the Department of Chemistry, SAS deserves special appreciation for their tireless efforts in making this conference a grand success, with the generous support from ANRF and other esteem sponsors.

I convey my best wishes to all the participants and sincerely hope that your time at VIT during this event will be enriching, productive, and fruitful.

With best wishes
Dr. G. Viswanathan
Founder & Chancellor

Dr. Sankar Viswanathan
Vice-President

MESSAGE

It would be our immense pleasure to have with us all the distinguished speakers, researchers, students, and participants from across the country and around the world during the prestigious International Conference on Organic and Inorganic Materials for Energy and Sustainability (ICMES-2026), organized by the Department of Chemistry, School of Advanced Sciences, VIT, Vellore.

I am sure that this conference will serve as an exceptional forum for young minds to interact with distinguished scientists, academicians, and industry experts under one roof. Such fruitful interactions enable young researchers to draw upon the experience and expertise of leading professionals, explore new scientific dimensions, and cultivate a strong scientific temper.

The conference will offer young scholars and students an excellent opportunity to showcase their research findings, exchange ideas, receive valuable feedback, and gain deeper insights into emerging developments in the field. These interactions will undoubtedly help nurture their creativity, strengthen their innovative skills, and inspire them to pursue impactful research.

This three-day scientific gathering will feature a series of engaging sessions with invited speakers from India and across the world, who will share their professional perspectives, research findings, knowledge, and experiences. I encourage all students, research scholars, faculty members, and participants to take advantage of this opportunity through active participation and discussion. Transformation of knowledge on such occasions benefit us and ultimately our nation as well.

Let us come together to exchange ideas, foster collaborations, ignite and inspire young minds, and work collectively towards making India a strong global hub for scientific research, innovation, and technological advancement.

With all good wishes,

Dr. SEKAR VISWANATHAN, PhD
Vice President

MESSAGE

I am delighted to learn that you will be participating in the International Conference on Organic and Inorganic Materials for Energy and Sustainability (ICMES-2026), organized by the Department of Chemistry, School of Advanced Sciences, VIT, Vellore. The conference offers a valuable platform for students and young researchers to interact with distinguished scientists, academicians, and experts from leading universities and research institutions across India and around the world.

I am confident that this three-day scientific gathering will bring out the best in our students and research scholars by providing them with opportunities to learn from and engage with some of the leading scientists and industry experts working in the areas of organic and inorganic materials for energy and sustainability. I encourage all participants to make the most of these interactions, exchange ideas, seek expert perspectives, and explore new avenues for research and innovation.

The conference also provides an excellent opportunity to interact with our faculty members from the Department of Chemistry, learn about the latest research activities and expertise within the department, and explore our advanced research facilities. I hope these interactions will pave the way for meaningful academic and research collaborations in the future.

I warmly congratulate all those who are presenting their research through oral and poster presentations. I also extend my heartfelt congratulations to the prize winners for their outstanding contributions and achievements.

I wish you all a memorable, enriching, and successful conference at VIT, Vellore.

With all my best wishes,

Dr. Sekar Viswanathan

Dr. Sandhya Pentareddy
Executive Director, VIT Vellore

MESSAGE

I am pleased to welcome you all to the International Conference on Organic and Inorganic Materials for Energy and Sustainability (ICMES-2026), organized by the Department of Chemistry, School of Advanced Sciences, VIT, Vellore. It gives me immense pleasure to extend a very warm welcome to all the delegates, scientists, academicians, and students.

This conference is a confluence of scientists and researchers coming together to share their knowledge, ideas, and new findings on a common platform. This gathering provides a valuable chance for students and young researchers to meet and talk directly with scientists and professors from India and other countries, eventually enabling the transfer of knowledge to the next generation of scientists and engineers.

ICMES-2026 organizers have invited 30 renowned delegates, who will deliver lectures covering topics that are critical for energy and sustainability. Young scholars will present their research findings through oral/poster presentations, and "best presentation" prizes, which are sponsored by publishers like RSC, and ACS, will be awarded. Thus, this platform will encourage them to do even better in the future.

On behalf of the organizers and the chemistry faculty, SAS, I express a warm welcome to all the delegates, speakers, and participants who accepted our invitation to come and make the conference a success. I hope everyone has three days of productive scientific endeavors that will shape a future-ready society.

Best wishes,

Dr. Sandhya Pentareddy

Ms. Kadhambari S. Viswanathan
Assistant Vice-President, VIT Vellore

MESSAGE

I am quite delighted to welcome you all to the International Conference on Organic and Inorganic Materials for Energy and Sustainability (ICMES-2026), organized by the Department of Chemistry, School of Advanced Sciences, VIT, Vellore. A very warm welcome to all the distinguished delegates, scientists, academicians, research scholars, and students.

This conference brings together all prominent scientific minds from across India and around the globe to share their knowledge, experience, expertise and recent findings in organic and inorganic materials relevant to energy and sustainability, thus paving the way for further exploration and new dimensions in related research areas.

The organizers of ICMES-2026 have invited 30 renowned scientists and experts for delivering lectures that cover a wide range of topics pertaining to energy and sustainability. Young scholars will also present their research findings through oral and poster presentations. To recognize and encourage their outstanding contributions, Best Presentation and Best Poster Awards, sponsored by organizations of repute and publishers such as the RSC and ACS, will be presented.

On behalf of the organizers and the faculty members of the Department of Chemistry, School of Advanced Sciences, I once again extend a hearty welcome to all the delegates, speakers, and participants who join us, accepting our invitation, to make this conference a grand success.

I hope that everyone will have three days of productive scientific discussions, fruitful interactions, and meaningful exchange of ideas, which will contribute to the advancement of science and technology and help shape a sustainable and future-ready society.

Best Wishes,

Dr. (Mrs.) V.S. Kanchana Bhaaskaran
Vice-Chancellor

MESSAGE

The convergence of science and engineering plays a vital role in shaping a better, safer, and more sustainable world. Scientific conferences provide a valuable platform for experts, researchers, and young scholars to share knowledge, exchange ideas, discuss emerging developments, and explore new frontiers of research. Such interactions foster collaboration and inspire the next generation of scientists and engineers.

It gives me immense pleasure that the Department of Chemistry, School of Advanced Sciences, VIT, Vellore, is organizing the International Conference on Organic and Inorganic Materials for Energy and Sustainability (ICMES-2026). I warmly welcome all the distinguished delegates, invited speakers, researchers, faculty members, students, and participants to this important academic gathering.

I sincerely appreciate the eminent speakers from India and abroad for sharing their expertise and latest research in areas including advanced functional materials, energy materials, nanomaterials, MOFs, COFs, drug design and medicinal chemistry, green and sustainable chemistry, environmental remediation, and other emerging fields.

I am particularly pleased that the conference provides young researchers with opportunities to present their work through oral and poster presentations, interact with experts, receive valuable feedback, and establish new collaborations. The Best Oral and Poster Presentation Awards, supported by the Royal Society of Chemistry (RSC) and the American Chemical Society (ACS), will further encourage young researchers to pursue excellence in their scientific endeavours.

I am confident that ICMES-2026 will promote meaningful scientific exchange, interdisciplinary collaboration, and innovative approaches towards addressing global challenges in energy and sustainability.

My best wishes to all the participants for a productive, enriching, and inspiring conference!

Partha Sharathi Mallick, Ph.D.,
Pro-Vice Chancellor

MESSAGE

I welcome all to the International Conference on Organic and Inorganic Materials for Energy and Sustainability (ICMES-2026), organised by the Department of Chemistry at the School of Advanced Sciences, Vellore Institute of Technology, Vellore.

I believe this conference will serve as a valuable platform for uniting students, research scholars, and researchers working on organic and inorganic materials to deliberate and explore ways to establish a sustainable future.

I would like to thank all the speakers and participants, both from India and abroad, for accepting our invitation and sharing their expertise at the conference. I am confident that this event will create opportunities for students, young researchers, professors, and scientists to network and collaborate on new research initiatives.

I also extend my gratitude to all the sponsors and well-wishers who helped the conference in many ways. I hope that this event will create opportunities for new partnerships between VIT and other organisations.

I wish the conference a great success.

Partha Sharathi Mallick

Dr. T. Jayabarathi
Registrar

MESSAGE

I am pleased to learn that the Department of Chemistry, School of Advanced Sciences, VIT, Vellore, is organising the International Conference on Organic and Inorganic Materials for Energy and Sustainability (ICMES-2026). It gives me immense pleasure to extend my warmest welcome to all the delegates, invited speakers, participants, research scholars, and students attending this conference.

The conference brings together experts and researchers from India and abroad and features around 30 invited talks by specialists working in diverse areas of chemistry and materials science. The central themes of energy and sustainability are not only fascinating from a fundamental science perspective but also highly relevant to the pressing energy challenges the world faces today. Advances in these areas are essential to developing innovative, sustainable solutions for the future.

I am also delighted that leading scientific organisations and publishers, including the American Chemical Society (ACS) and the Royal Society of Chemistry (RSC), are supporting the conference by recognising young scientists' research contributions through awards for the Best Poster and Oral Presentations. Such initiatives will certainly encourage research scholars and young researchers to pursue innovative and impactful research.

On behalf of the organisers, I extend my sincere greetings and a very warm welcome to all the delegates and participants who have accepted our invitation and joined us for ICMES-2026. Your presence and valuable contributions will play an important role in making this conference a great success.

I am confident that ICMES-2026 will create a vibrant atmosphere for scientific discussion, idea exchange, networking, and collaboration, while inspiring the next generation of scientists and contributing to the advancement of science and the betterment of society.

Best wishes,

Dr. T. Jayabarathi

Dr. *Karthikeyan K.*
Dean, School of Advanced Sciences
VIT Vellore

MESSAGE

It gives me great pleasure to know that the Department of Chemistry, School of Advanced Sciences, VIT, Vellore, is organizing the International Conference on Organic and Inorganic Materials for Energy and Sustainability (ICMES-2026). On behalf of the School of Advanced Sciences, I extend a very warm welcome to all delegates, invited speakers, participants, research scholars, and students joining this conference.

This conference brings together nearly 30 eminent speakers from India and abroad, working across diverse frontiers of chemistry and materials science, with a shared focus on energy and sustainability — themes that are central to addressing some of the most pressing scientific and societal challenges of our time. The School takes great pride in fostering research environments that encourage such meaningful academic exchange.

I am glad that esteemed organizations such as the American Chemical Society (ACS) and the Royal Society of Chemistry (RSC) are supporting ICMES-2026 by recognizing outstanding contributions of young researchers through Best Poster and Oral Presentation awards. Such recognition will go a long way in motivating our young scientists to pursue impactful and innovative research.

I extend my heartfelt greetings to all participants and wish ICMES-2026 great success. I am confident that this conference will provide a stimulating platform for scientific discussion, collaboration, and the exchange of new ideas, while inspiring the next generation of researchers.

With regards,

Dr. *D Rajan Babu*
Professor & Associate Dean
School of Advanced Sciences
VIT, Vellore

MESSAGE

It is a matter of great pride and pleasure for me to learn that the Department of Chemistry, School of Advanced Sciences, VIT, Vellore, is hosting the International Conference on Organic and Inorganic Materials for Energy and Sustainability (ICMES-2026). I take this opportunity to extend my warmest welcome to all the distinguished delegates, invited speakers, participants, research scholars, and students attending this important scientific gathering.

Nearly 30 eminent researchers from India and abroad are participating in ICMES-2026 and sharing their latest research findings, expertise, and experiences. The conference promises a rich and diverse scientific programme focusing on energy and sustainability—areas of immense significance to both fundamental research and contemporary societal challenges. Conferences of this nature play a vital role in strengthening the research culture within our School and fostering meaningful interactions among the wider scientific community.

I am particularly pleased that prestigious organizations such as the American Chemical Society (ACS) and the Royal Society of Chemistry (RSC) are supporting this conference and encouraging young researchers by recognizing their scientific contributions through Best Poster and Best Oral Presentation Awards. Such initiatives are highly valuable in motivating young scientists to pursue excellence and contribute meaningfully to the advancement of science.

I convey my warm greetings and best wishes to all the participants and organizers of ICMES-2026. I am confident that this conference will provide an excellent platform for scientific exchange, collaboration, and the sharing of innovative ideas, while inspiring the next generation of researchers in chemistry and materials science.

I wish ICMES-2026 a grand success and a memorable and intellectually enriching experience for all.

With best regards,

D. Rajan

Dr. Karpagam S
HOD, Department of Chemistry, SAS
VIT Vellore

MESSAGE

It is with great pleasure that I extend my warmest welcome to all the distinguished delegates, invited speakers, participants, research scholars, and students attending the International Conference on Organic and Inorganic Materials for Energy and Sustainability (ICMES-2026), organized by the Department of Chemistry, School of Advanced Sciences, VIT, Vellore.

Our Department takes immense pride in bringing together nearly 30 distinguished researchers and speakers from India and abroad to share their latest research findings and deliberate on the important themes of energy and sustainability—areas that are at the forefront of contemporary research in chemistry and materials science. This conference reflects our Department's continued commitment to promoting cutting-edge research, fostering international collaboration, and creating meaningful opportunities for scientific exchange.

I am particularly pleased that prestigious organizations such as the American Chemical Society (ACS) and the Royal Society of Chemistry (RSC) are supporting ICMES-2026 and encouraging young researchers by recognizing their achievements through Best Poster and Best Oral Presentation Awards. Such initiatives will undoubtedly motivate our research scholars and young faculty members to pursue excellence and make significant contributions to their respective fields. We are also deeply grateful to all our sponsors for their generous support and valuable contribution towards making this conference possible. Their encouragement and partnership are greatly appreciated.

On behalf of the Department of Chemistry, I extend my heartfelt welcome and best wishes to all the delegates, speakers, participants, research scholars, and students. I wish ICMES-2026 every success and hope that all of you will have a scientifically enriching and memorable experience.

Best wishes,

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PL-1

Dr. R. VIJAY
Director
Institute: **International Advanced Research Centre for Powder Metallurgy & New Materials (ARCI)**
Address: Balapur P.O., Hyderabad - 500005
Contact Number: 040-29561681
e-Mail: director@arci.res.in

Dr. R. Vijay is the Director of the International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI), an autonomous R&D Centre under the Department of Science and Technology, Government of India. With over three decades of experience in advanced materials research and technology development, since 1994, joining as a Scientist and rising through the ranks to become the Director of the institute.

He holds a B.Tech. and M.Tech. in Chemical Engineering from the National Institute of Technology, Warangal, and a Ph.D. in Mechanical Engineering from the Indian Institute of Technology Madras, where his research focused on hydrogen storage in magnesium-based materials.

Dr. Vijay's research spans a wide range of advanced materials and emerging technologies, including nanomaterials, mechanical alloying, oxide dispersion strengthened steels, energy storage materials including Li-ion and Na-ion batteries, supercapacitors, biomaterials, additive manufacturing, and hydrogen generation and storage. He has played a pivotal role in translating research into industrial applications, successfully transferring multiple technologies to industry, notably lithium iron phosphate (LFP) cathode materials for batteries, silica aerogel insulation, tungsten-based defence components, lead-free bearing alloys, and heat pipe technologies.

Over his career, he has led several major national and international research projects funded by agencies such as DST, DRDO, ANRF, MNRE, and through international collaborative programmes under IGSTC and GITA. He has contributed significantly to scientific literature with over 67 peer-reviewed publications and holds 30 national and international patents.

Dr. Vijay has received several prestigious recognitions, including the MRSI Materials Science Annual Prize, the Distinguished Alumnus Award from NIT Warangal, the Engineer of the Year Award from Institution of Engineers and Govt. of Andhra Pradesh, and the FTCCI Excellence Award for Individual Achievement in Science and Engineering. He is a Fellow of The Institution of Engineers (India) and the Telangana Academy of Sciences, and was conferred the ASTC Honorary Fellow by the Academy of Science, Technology and Communication (ASTC), Hyderabad.

In addition to his research leadership, he serves in several academic and advisory capacities, including as a Senate Member of the Indian Institute of Technology Tirupati, Member of the Scientific and Research Advisory Committee of the Kotak School of Sustainability at the Indian Institute of Technology Kanpur, Adjunct Professor at the University of Hyderabad, Member of the NIT Warangal Development Board, and Governing Council Member of the National Centre for Additive Manufacturing.

Under his leadership, ARCI continues to strengthen its position as a premier materials R&D Centre, advancing cutting-edge technologies with a strong emphasis on industrial relevance, translational research, technology transfer, and national mission objectives.

Advanced Materials and Technologies for Sustainable Energy and a Self-Reliant India

Dr. R. Vijay

Director, International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI), Hyderabad

An Autonomous R&D Centre of the Department of Science & Technology, Government of India

Abstract:

The transition towards a sustainable energy future and a self-reliant India requires not only new sources of energy, but also advanced materials and indigenous technologies that can efficiently convert, store and utilize energy. Materials science and engineering therefore lie at the heart of the global transition towards clean energy, enabling innovations ranging from solar energy conversion and electrochemical energy storage to hydrogen technologies and engineered coatings, thus addressing the challenges of resource sustainability and scalable manufacturing.

ARCI embarked on major programmes for development and demonstration of materials technologies for batteries (Li-ion, Na-ion, Li-S and solid-state batteries), solar energy and hydrogen generation.

The talk focuses on the journey adopted to take the above-mentioned technologies from Lab to Market.

PL-2

Dr. Jörg J. Schneider

Department: Department of Chemistry
Institute: Institute of Inorganic Chemistry
Address: Peter-Grünberg-Str. 12
Contact Number:
e-Mail: joerg.schneider@tu-darmstadt.de

Prof. Dr. Jörg J. Schneider

Jörg J. Schneider studied chemistry at the Philipps Universität Marburg, Germany, and obtained a Dr. rer. nat. degree in 1986. From 1987 until 1988 he received a Fulbright fellowship and was post doc at Kansas State University, KS, Manhattan, USA and from 1989 -1994 post-doc and junior group leader at the Max-Planck-Institut für Kohlenforschung, Mülheim a.d. Ruhr, Germany. From 1994 until 1999 he was Heisenberg Fellow of the Deutsche Forschungsgemeinschaft, DFG, and Lecturer at the Inorganic Chemistry Department at the University of Essen, from 1999 - 2000 temporary professor for Inorganic Chemistry there and from 2000 - 2003 full professor for Inorganic Chemistry at the Karl-Franzens-Universität, Graz, Austria. Since 2003 he has been a full professor for Inorganic and Mesoscopic Chemistry at the Technische Universität Darmstadt, Germany.

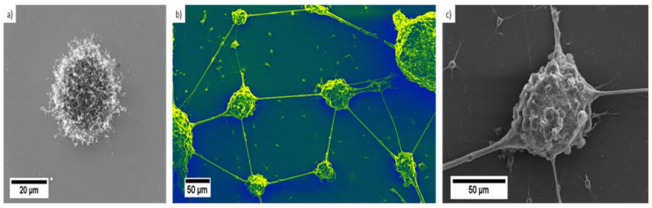
His research interests span different areas of materials chemistry focussing on functional properties and application of carbon nanotubes, graphene, metal oxides for electronics, sensing (gas and electromechanical sensing) heterogeneous catalysis and as well as energy applications (gas storage and batteries). As he is originally trained and scientifically raised as an organometallic chemist. Long standing and still ongoing interests but over the years becoming minor in scope are in the field organometallic chemistry e.g. of polycondensed aromatics and free metal atom chemistry.

Inorganic functional materials for sensing, catalysis and electronics

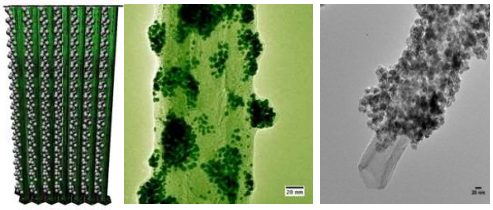
Jörg J. Schneider*, Technical University Darmstadt, Department of Chemistry, Inorganic Chemistry, Peter-Grünberg Str.1, 64287 Darmstadt, Germany
joerg.schneider@tu-darmstadt.de

Abstract:
I will present selected work on inorganic nanomaterials ranging from carbon nanomaterials to metal oxides which we have performed over the last 30 years in these areas at different research environments.[1-4] The lecture starts with encompassing fundamental work on graphitic carbon nanotubes (CNTs), their synthesis and application as sensors as well as studies on gas adsorption of these nanomaterials. This is followed by a fresh view into synthesis and characterization of single atom catalysts which can be approached by a unique low temperature approach. In the final part of the lecture I will present our long standing research into semiconducting metal oxides, their synthesis, characterization and application as field effect transistor materials.

Figures:



a) neuron cells grown on CNTs [1,2,3]
b) neuron cell network on CNT [1,2,3]
c) single neuron on CNTs with axons [1,2,3]



a) schematic of ZnO particles on VA-CNTs[4]
b) SEM of ZnO nanoparticles on VA-CNTs [4]
c) TEM of ZnO particles on a single CNT [4]

References and Notes:

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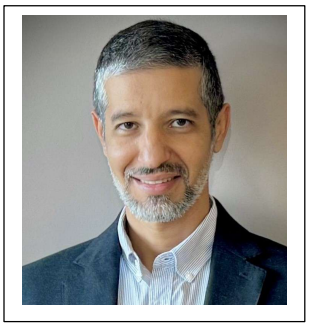
3. Koerbitzer, B.; Krauss, P.; Nick, C.; Schneider, J.J.; Thielemann, C.; *2D Mater.* **2016**, 3, 024004
4. Okeil, S.; Dönges, I.; Pfleger, S.; Krausmann, J.; Schneider J.J.; *Dalton Trans*. **2017**, 46, 5189-5201

PL-3

Dr. Zakaria Halime
CNRS Research Director

Department: Bioinorganic Chemistry
Institute: Institut de Chimie Moléculaire et des Matériaux d'Orsay
Address: 19 Avenue des Sciences, 91400, Orsay, France.
Contact Number: +33777893380
e-Mail: zakaria.halime@universite-paris-saclay.fr



Dr. Zakaria HALIME is a CNRS Research Director at the Institute of Molecular and Material Chemistry of Orsay (ICMMO, Université Paris-Saclay) and his expertise lies in artificial photosynthesis. He earned his bachelor's degree in chemistry from Sidi Mohamed Ben Abdellah University (Fès, Morocco) in 2002, followed by a Ph.D. in Chemistry from Université de Rennes 1 (France) in 2006 under the supervision of Dr. Bernard BOITREL. He conducted postdoctoral research at Johns Hopkins University (USA, Prof. K. D. Karlin's group) and Osaka University (Japan, Prof. S. Fukuzumi's lab). His career includes roles as a scientific advisor at Wells Fargo (USA) and co-founder/CEO of Easy Chelators (France), a company focused on radiopharmaceuticals. His current research focuses on the activation and transformation of small molecules (CO_2, O_2, H_2, H_2O, *etc.*) to advance sustainable chemistry and clean energy solutions.

Bio-inspired Design for Catalytic CO_2 Reduction

Zakaria Halime*
Université Paris-Saclay, CNRS, Institut de Chimie Moléculaire et des Matériaux d'Orsay, 91400, Orsay, France.

Abstract: Rational strategies for catalyst design and improvement hinge on what we continually learn from natural systems, as they exhibit exceptional stabilities and performance. Carbon monoxide dehydrogenase (CODH) stands as the typical inspiration for scientists working in the field of CO_2 reduction as it is known to catalyze the reversible reduction of CO_2 to CO (see Figure).[1] Lessons from the structure and functions of this enzyme point out to some important findings that can be artificially mimicked by catalyst design: (1) precisely positioned amino acid residues to induce electrostatic or hydrogen-bonding interactions with the CO_2 substrate, (2) a bifunctional activation of CO_2 substrate by two metal centers, (3) an iron-sulfur cluster acting as an electronic relay and buffer to the catalytic unit. Implementing some of these functionalities in the second coordination sphere of an iron-porphyrin catalyst has successfully led to significantly decrease the overpotential while improving the selectivity as well as the catalytic turnover numbers (TONs) and frequencies (TOFs) of homogeneous[2,3] and heterogeneous[4,5] CO_2 to CO reduction reaction.

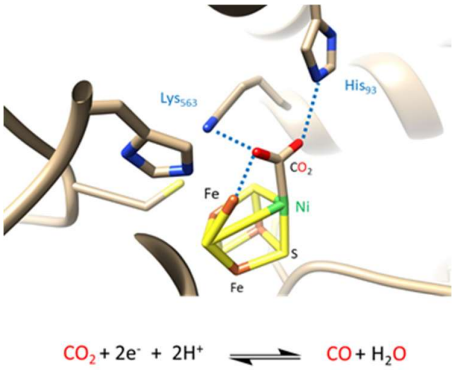


Figure: Carbon monoxide dehydrogenase (CODH) active site and its corresponding reaction.

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PL-4

Dr. Balaji R. Jagirdar
Professor

Department: Inorganic & Physical Chemistry
Institute: Indian Institute of Science
Address: Bangalore 560 012, India
Contact Number: 080-2293 2825
e-Mail: jagirdar@iisc.ac.in

Balaji Jagirdar obtained his M.Sc. in Chemistry from IIT-Bombay in 1989 and his Ph.D. degree in Chemistry from Kansas State University in 1994. He had a year and a half stint as a postdoc at the University of Colorado, Boulder during 1994-'95 before returning back to India in Oct 1995 and joined the faculty of the Dept of Inorganic & Physical Chemistry at Indian Institute of Science, Bangalore, India. He joined as a lecturer and rose to the rank of a full professor in 2011. His research interests include activation of small molecules using organometallic compounds, homogeneous and heterogeneous catalysis, and materials for hydrogen storage and generation. He served as a member of the Editorial Advisory Board of Dalton Transactions for several years. He served as the Associate Dean of the Undergraduate Program at IISc during 2015-2018 and as the Dean, during 2020-2024. Presently, he is the Editor-in-Chief of Journal of Chemical Sciences.

Digestive ripening facilitated nanoengineering of diverse nanostructured materials

*Balaji R. Jagirdar**
Department of Inorganic & Physical Chemistry, Indian Institute of Science, Bangalore 560012, India; jagirdar@iisc.ac.in

Abstract: Solvated metal atom dispersion (SMAD) together with digestive ripening transform colloids comprised of metal nanoparticles of broad size distribution, nearly monodisperse. Our group exploited the strengths of this combination of synthetic methodologies to realize nearly monodisperse nanoparticles of a wide variety of metals (Mg, Ca, Mn, Fe, Co, Pd, Cu, Ag, Au, Al, In, and Eu) in the past.

Bimetallic nanostructures of metals are especially interesting as they exhibit synergistic properties arising from their monometallic counterparts and hence, offer the possibility to integrate and modulate them as required. Co-digestive ripening has emerged as an excellent synthetic strategy to realize shape and size-controlled colloidal bimetallic nanostructures. In this regard, our group prepared a wide array of bimetallic heterostructures such as core-shell, composites, alloy, intermetallic and Janus nanoparticles using this strategy. Detailed mechanistic insights into the formation of such novel structures have also been established. Some of the bimetallic nanosystems prepared by co-digestive ripening method displayed exquisite catalytic activities bringing out the synergism of the constituents of such systems. Co-digestive ripening has recently been exploited to realize a homogeneous ternary nanosystem as well, under mild reactive conditions. Efforts are in progress presently in our laboratories to extend this novel methodology to include the synthesis of high-entropy alloy nanostructured materials. Additionally, applications of some of the materials synthesized using this methodology in the fields of hydrogen storage and generation, magnetism, catalysis, and surface enhanced Raman spectroscopy will also be discussed.

PL-5

Prof. Dr. Hiroshi Kitagawa

Department: Division of Chemistry, Graduate School of Science
Institute: Kyoto University
Address: Kitashirakawa-Oiwakecho, Sakyo, Kyoto 606-8502, Japan
Contact Number: +81-75-753-4035
e-Mail: Kitagawa.hiroshi.8v@kyoto-u.ac.jp

Hiroshi Kitagawa, born in Osaka in 1961, received his Ph.D. from Kyoto University in 1992 and, after working as an assistant professor at the Institute for Molecular Science (IMS), as a visiting researcher under supervision of Prof. Peter Day, Davy-Faraday Research Laboratory, Royal Institution of Great Britain, and as an assistant professor at the Japan Advanced Institute of Science and Technology (JAIST), was appointed as associate professor at the University of Tsukuba in 2000. He became a professor at Kyushu University in 2003 and returned to Kyoto University in 2009. He was employed at the Japan Science and Technology Agency (JST) as Director of "Science and Creation of Innovative Catalysts" and is now employed at JST as Director of "Exploring Innovative Materials in Unknown Search Space" and as Program Officer of the Materials Science Panel, Fusion Oriented Research for Disruptive Science and Technology. He is also Programme Officer (Materials), LOTUS Programme, Japan Science and Technology Agency (JST). He was also Chief Program Officer in Chemistry Group, Japan Society for the Promotion of Science (JSPS) from 2020 to 2024. He is a previous President of the Japan Society of Coordination Chemistry from 2020 to 2024. He is now Executive Director, Japan Synchrotron Radiation Research Institute (JASRI/SPring-8). He is also Vice Provost of Kyoto University for Planning and Strategy Coordination and is to be Provost of Kyoto University from October, 2026. He has published more than 590 original research papers on solid-state chemistry, coordination chemistry, nanoscience, low-dimensional electron systems and molecule-based conductors.

Modern Alchemy: Binary to High-Entropy Nano-alloys and Oxides

Hiroshi Kitagawa*
Division of Chemistry, Graduate School of Science, Kyoto University, Kitashirakawa-Oiwakecho, Sakyo-ku, Kyoto 606-8502, Japan

Abstract: Platinum group metal (PGM) nanoparticles (NPs) have been investigated in a variety of research fields such as catalysis and electronics. Among the types of alloys, solid-solution alloy NPs have the advantage of being capable of continuously changing their properties by tuning their composition. However, synthesizing PGM solid-solution alloy NPs with any combination and composition is not an easy task due to the metallurgical aspects. In this work, we have focused on PGM-based solid-solution alloy NPs, and particularly those with immiscible alloy systems[1-5].

The physical and chemical properties of most solids are strongly correlated to their electronic structure, particularly the DOS at the E_F. In 2015, our group proposed the "DOS engineering" concept for designing materials[4], which calls for the control not only of the location of the d-band center, but also of a suitable DOS shape, such as the band width and the DOS shape of unoccupied and occupied stated around E_F. We propose that by means of "interelement fusion," as shown in **Figure** where the elemental periodic table is colored by the *s*, *p*, *d*, and *f* groups, it is possible to manipulate the shape of the DOS freely by choosing elements from the *s*, *p*, *d*, and *f* groups according to the properties desired. Our recent development of the synthetic methods are also introduced.

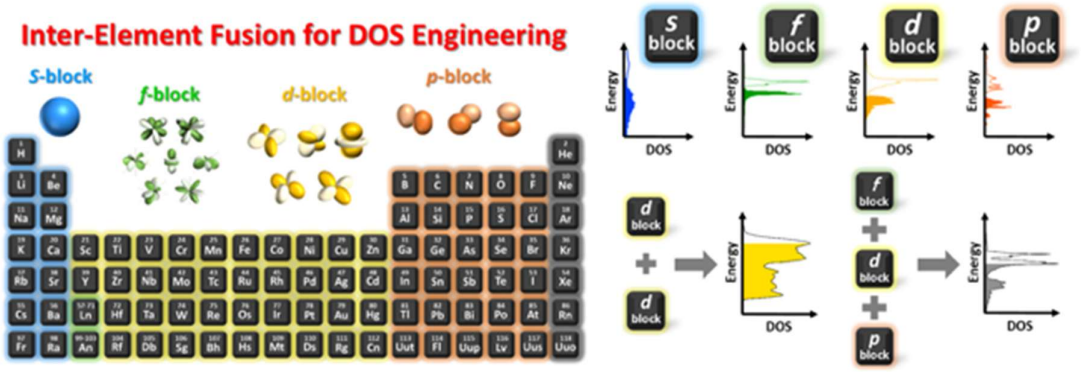

Figure. Our proposed concept for element strategy, density-of-state engineering by inter-element-fusion by. using *s*-, *p*-, *d*-, and *f*-blocks elements.

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Keynote Lecture- KL

KL-1

Dr. Rowan D. Young
ARC Future Fellow and Associate Professor

Department: School of Chemistry and Molecular Biosciences
Institute: University of Queensland
Address: 68 Cooper Road, St Lucia Queensland 4067, Australia
Contact Number: NA
e-Mail: rowan.young@uq.edu.au

Rowan is an Associate Professor and ARC Future Fellow at the University of Queensland in Australia. He obtained his PhD at the Australian National University's Research School of Chemistry where he was awarded the Director's Prize in 2012. After post-doctoral stints at the University of Oxford and the University of Edinburgh, he began his independent career at the National University of Singapore in 2014 before relocating to the University of Queensland in 2023. His research is primarily focused on methodology development using pincer complexes and frustrated Lewis pairs to address challenges in small molecule activation. His achievements have been recognized with research awards including the Thieme Chemistry Journal Award, the Asian Chemistry Prize in Organic Chemistry and an ARC Future Fellowship.

Developing Chemistry for a Closed Fluorine Economy

Rowan D. Young
The University of Queensland, Brisbane, Australia 4067, rowan.young@uq.edu.au

Abstract: Fluorinated molecules are critical components of many advanced technologies.[1] Fluorine underpins basic technologies in pharmaceuticals, medical imaging, agrochemicals, refrigeration, advanced polymers, nuclear fuel enrichment, lithium-ion batteries and metal refining. At the same time, a number of fluorine containing molecules have become known as hazardous chemicals to the environment and to our health.[2] Indeed, the basic synthons of fluorine, HF and F_2, are extremely toxic and dangerous.

Given the unique characteristics of fluorine and fluorinated compounds, our efforts as chemists should be focused on developing methods of reusing and recycling fluorinated compounds rather than prohibiting them. As a society we have amassed megatons of fluorocarbon waste that cannot be released to the environment and is difficult to destroy. If suitable chemical methods are developed, this waste would become a valuable reservoir of fluorine for reuse in the fluorochemical industry.

Over the last 10 years, my group has been focused on developing methods to allow the chemical reuse of fluorocarbons. I will share efforts we have made and describe the unique chemistry that is possible through selective and/or targeted defluorination of polyfluorocarbons (Figure 1).[3]

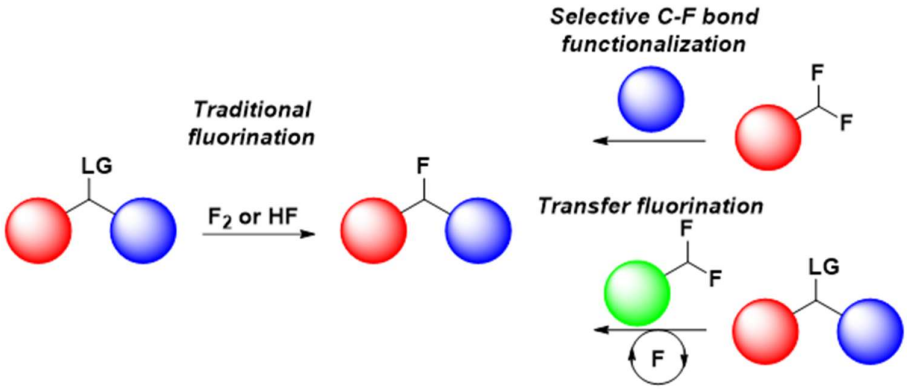

Figure 1: Selective defluorination and transfer fluorination provide powerful chemical strategies to avoid the use of hazardous fluorine synthons.

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KL-2

Prof. Dr. C V S Brahmananda Rao
Head, Fuel Chemistry Division and Dean (Chemistry), HBNI-IGCAR
Department: Department of Atomic Energy
Institute: Indira Gandhi Centre for Atomic Research
Address: Kalpakkam 603102, Tamil Nadu
Contact Number: 9444886144
E-Mail: brahma@igcar.gov.in

Prof. Rao did his graduation in BSc. Chemistry (Hons.) from Delhi University and post-graduation in chemistry from University of Hyderabad and Joined 38th batch of BARC Training School in 1994. After training he joined Radiochemistry Laboratory at IGCAR in 1995. He did his Ph.D. from Madras University in the field of organic ligand synthesis and its application for the recovery of actinides. He is head of in Fuel Chemistry Division at IGCAR.

He has o**ver 150 publications in journals, seminars and symposia.**

He is also Dean of Chemical Sciences at IGCAR in Homi Bhabha National Institute, Mumbai.

His field of interest includes synthetic organic chemistry, d**evelopment of alternate extractants for actinide separation and recovery, computational chemistry and high temperature mass spectrometry**.

Application of Metal Organic Frameworks in Nuclear Industry

C.V.S. Brahmananda Rao
Head, Fuel Chemistry Division and Dean, Chemical Sciences (HBNI)
Indira Gandhi Centre for Atomic Research, Kalpakkam

Abstract:
Metal–organic frameworks (MOFs) are a class of crystalline porous materials having high surface areas, tunable pore structures, ordered channels, and chemically adjustable functionalities, making them promising materials for selective actinide sorption. Post-synthetic modification (PSM) further enables the introduction of specific donor groups without completely reconstructing the parent framework. Various metal organic frameworks (MOFs) containing different metal ions and organic linkers were synthesized by solvothermal method and PSM was carried to synthesize MOFs containing different functional groups. The MOFs were characterized by Fourier transform infrared spectroscopy (FTIR), Powder XRD, BET surface area analysis, Thermogravimetric analysis (TGA), NMR (^{13}C, ^{1}H and ^{31}P), Scanning Electron Microscopy (SEM), and Energy Dispersive X-ray spectroscopy (EDX). MOFs were examined for different applications such as for recovery of uranium from sea water, recovery of thorium from aqueous solutions. The efficient separation and recovery of actinides from aqueous systems is an important requirement in nuclear fuel-cycle operations, radioactive waste management, environmental remediation, and resource recovery. Uranium and thorium are particularly important actinides because of their roles in nuclear energy and their potential occurrence in mining effluents, process streams and contaminated water. This talk provides an overview of MOFs for actinide sorption, covering their structural features, important properties, synthesis methods, post-synthetic functionalization, actinide chemistry, sorption mechanisms, and characterization approaches. Fluorescence sensing studies were carried out with MOFs for sensing of different metal ions such as uranium and fission products. The nature of U(VI) interactions on MOFs were investigated by applying density functional theory (DFT). MOFs were also examined as phosphors for light emitting diodes. MOFs were also examined for storage of hydrogen.

KL-3

Dr. S. Nagarajan
Designation: Professor

Department: Chemistry
Institute: Central University of Tamil Nadu
Address: Thiruvarur- 610 005
Contact Number: 9443046272
e-Mail: snagarajan@cutn.ac.in

Prof. S. Nagarajan has been associated with the Central University of Tamil Nadu (CUTN) since 2012, when he joined the University as the first faculty member of the Department of Chemistry. As the founding Head of the Department, he played a seminal role in establishing and advancing its academic, teaching, and research programmes, thereby laying a strong foundation for its sustained growth and development. His academic leadership at the University has been marked by a series of significant administrative responsibilities. He has served as Dean, School of Basic and Applied Sciences; Dean, Students' Welfare; and Controller of Examinations. In recognition of his academic experience and institutional leadership, he currently serves as the Dean of Academics at CUTN.

His academic foundation is rooted in Tamil Nadu, beginning with an MSc Organic Chemistry and a PhD from Annamalai University. His expertise and commitment to research earned him global recognition through prestigious international assignments, including a Postdoctoral Fellowship at the Nanoscience Group of CEMES-CNRS in Toulouse, France, and a Guest Researcher position at the International Center for Materials Nano-architectonics (MANA) at NIMS in Tsukuba, Japan. Prof. Nagarajan has been honored with several notable distinctions, including the BOYSCAST Fellowship from the Ministry of Science and Technology, Government of India; the Young Scientist Fellowship from the Tamil Nadu State Council for Science and Technology; and the CSIR Research Fellowship in New Delhi. He is also a Fellow of the Royal Society of Chemistry (FRSC), Fellow of the Indian Chemical Society, and Fellow of the Academy of Sciences, Chennai, reflecting his stature in the scientific community. He has supervised 16 PhD scholars and is presently guiding 8 scholars, 22 MPhil researchers, and three Postdoctoral Fellows, contributing significantly to the next generation of scientific talent. He published 139 research papers in international journals.

His research productivity and leadership have attracted competitive funding from premier agencies, including ANRF, DST, CSIR, UGC, and industry partners, further establishing his reputation as a leading scientist and academic leader.

Research areas:
Organic Synthesis & Organic Electronic Materials.

Molecular Engineering of Donor–Acceptor Architectures for Multilevel Resistive Memory Device Applications

S. Nagarajan
Department of Chemistry, Central University of Tamil Nadu, Thiruvarur- 610 005, India

Abstract:
The development of high-density organic resistive memory devices with reliable multilevel data-storage capability is of considerable interest for next-generation non-volatile memory technologies. A series of molecularly engineered bisphenanthro[9,10-d]imidazole-based donor–acceptor (D–A) systems was synthesized for solution-processable write-once-read-many (WORM) memory applications. The molecular architecture was systematically evolved from a mono-phenanthroimidazole D–A framework to bis-phenanthroimidazole-based acceptor–donor–acceptor (A–D–A) architectures to modulate intramolecular charge transfer, electronic coupling, and charge-trapping characteristics. The mono-phenanthroimidazole derivative exhibited binary WORM behavior with an ON/OFF current ratio of 10^5. Expansion of the π-conjugated acceptor framework to bis-phenanthroimidazole architectures substantially enhanced resistive-switching characteristics, which can be attributed to increased charge-trapping density and strengthened donor–acceptor interactions. Notably, incorporation of a quinoline auxiliary acceptor afforded the most pronounced performance, delivering stable ternary WORM switching with distinct OFF, ON1, and ON2 states and a high ON/OFF current ratio of 10^8. The devices demonstrated excellent operational stability, retaining their programmed states for more than 4000 s and exhibiting reliable read endurance over 100 cycles. These findings establish molecular control over donor–acceptor strength, π-conjugation, and spatially differentiated trap sites as an effective strategy for regulating binary-to-ternary resistive switching.

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Invited Lecture- IL

IL-1

Dr. C. Sivasankar
Designation: Professor
Department: Chemistry
Institute: Pondicherry University (A Central University)
Address: R. V. Nagar, Kalapet, Pondicherry 605014
Contact Number: +91 9442669711
e-Mail: siva.che@pondiuni.ac.in

Prof. Dr. C. Sivasankar completed his B.Sc. and M.Sc. degrees in Chemistry at the University of Madras, studying at Thirumagal Mills College, Gudiyattam, and Muthurangam Government Arts College, Vellore, respectively. He obtained his Ph.D. in Organometallic Chemistry from the Indian Institute of Science (IISc), Bangalore, under the guidance of Prof. Dr. A. G. Samuelson.

He subsequently pursued postdoctoral research at several internationally renowned institutions, including Christian-Albrechts-Universität zu Kiel, Germany, under Prof. F. Tuczek; Osaka University, Japan, under Prof. Hiroki Sasai; and The Scripps Research Institute (TSRI), USA, under Prof. R. A. Periana.

He is currently serving as a Professor in the Department of Chemistry at Pondicherry University. His research interests encompass **Catalysis, Organometallic Chemistry, Computational Chemistry, and Bioinorganic Chemistry**.

Prof. Dr. Sivasankar serves on the Editorial Board of *Scientific Reports* (Nature Portfolio) and is a reviewer for several leading journals published by the American Chemical Society (ACS), Royal Society of Chemistry (RSC), Wiley, and Elsevier. He is also serving as a Director of Pondicherry University Start-up Center.

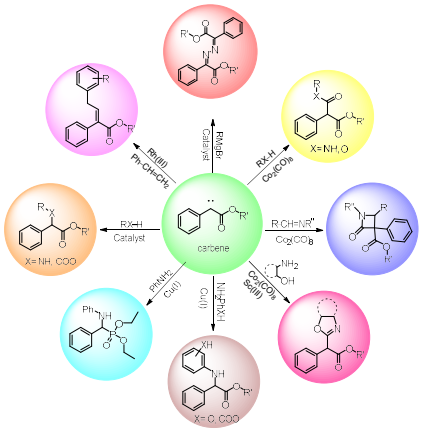
In recognition of his contributions to chemistry, he has been awarded the **Bronze Medal by the Chemical Research Society of India (CRSI)** and has been elected a **Fellow of the Royal Society of Chemistry (FRSC), London**.

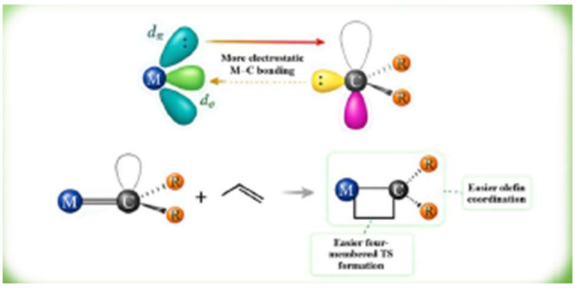
Transition-Metal-Complex-Catalyzed Carbene Chemistry for Organic Synthesis: Experimental and DFT Studies

Chinnappan Sivasankar*

Department of Chemistry, Pondicherry University (A Central University), R.V. Nagar, Kalapet, Pondicherry 605014, INDIA

Abstract: We have developed a series of novel strategies for carbene-insertion reactions into X–H bonds (X = C, N, O, and S) using transition-metal catalysts, enabling the efficient synthesis of a range of biologically important scaffolds, including α-amino esters, α-acyloxy esters, and β-unsaturated α-esters. We have also reported the symmetric homocoupling of diazo compounds in the presence of RMgX reagents to furnish diazines, which have potential applications in the sensing of toxic metal ions. Furthermore, we have employed [$Co_2(CO)_8$] as both a catalyst and a solid CO source for the generation of ketenes from diazo compounds. This approach has enabled the development of versatile synthetic methodologies for the preparation of α-amido esters, diesters, β-lactams, benzoxazoles, and related structures. Driven by our interest in carbene chemistry, we have also investigated the bonding characteristics of metal–carbene bonds in olefin-metathesis catalysts.





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IL-2

Dr. C. Gunanathan
Professor and Chairperson
School of Chemical Sciences
NISER Bhubaneswar
e-Mail: gunanathan@niser.ac.in
Website: https://sites.google.com/view/gunanathan

Professional Experience

2022- Professor, NISER Bhubaneswar, India
2017- Associate Professor, NISER Bhubaneswar, India
2013- Reader F, NISER Bhubaneswar, India
2011- Assistant Professor, NISER Bhubaneswar, India
2011- Ramanujan Fellow (SERB), NISER Bhubaneswar, India
2009- Alexander von Humboldt Research Fellow, RWTH Aachen University, Germany
2006- Dean of Faculty Postdoctoral Fellow, Weizmann Institute of Science, Israel
2005- Postdoctoral Fellow, Weizmann Institute of Science, Israel

Education

2005 Ph. D Central Salt and Marine Chemicals Research Institute, Bhavnagar, India
1999 M. Sc Department of Organic Chemistry, University of Madras, India
1997 B. Sc RKM Vivekananda College, University of Madras, India

Awards and Recognitions

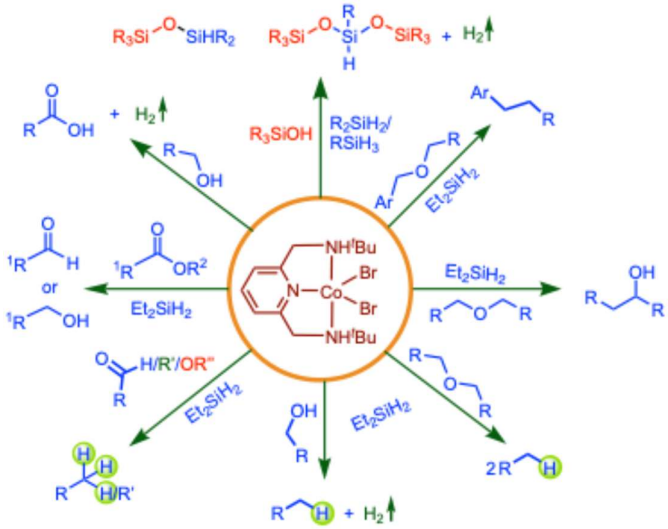
2026- *INSA Distinguished Lecture* Fellowship
2025- *Member, Board of Studies, JP College of Arts and Science*, Tenkasi-Nominee of Manonmaniam Sundaranar University (2025-2028)
2024-*INSA Associate Fellow* by Indian National Science Academy, New Delhi
2023-Convener, Board of Studies for *Integrated Master's* Program in Homi Bhabha National Institute, Mumbai
2023-Editorial Board Member of *Journal of Chemical Sciences*
2022-2024-Convener, Post-Graduate Committee, School of Chemical Sciences, NISER
2021-2024 - Co-opted member in SERB Expert Committee
2020-Top 3% highly cited author from India in American Chemical Society
2020-Thieme Chemistry Journals Award
2020-CRSI Bronze medal
2019 -Top Peer Reviewer Award by Publons
2016 -ECRP award -First Prize (10,000 Euro)

Research Interests: *Catalysis, Organometallic Chemistry, Reaction Mechanism, and Synthetic Methods.*

Cobalt Catalysis Enabled by Metal-Ligand Cooperation

Chidambaram Gunanathan*
School of Chemical Sciences, National Institute of Science Education and Research (NISER), An OCC of Homi Bhabha National Institute, Bhubaneswar-752050, India
*Corresponding Author E-mail: : gunanathan@niser.ac.in

Abstract: A new, simple and ready to access NNN^{Ht}Bu cobalt pincer complex was designed and prepared, which catalyzed selective synthesis of symmetrical disiloxanes, cyclosiloxanes, and cage like siloxanes from silanes and water, and unsymmetrical monohydro disiloxanes from silanes and silanols.[1] Cobalt pincer catalyzed acceptorless dehydrogenative oxidation of primary alcohols to carboxylic acids was reported.[2] Remarkably, Liberated H_2 is the only byproduct in these reactions. Cobalt pincer catalyzed selective synthesis of aldehydes and alcohols using hydrosilylation of esters was developed.[3] Interestingly, the same catalyst catalyses both transformations and the complete selectivity was attained by stoichiometry of diethylsilane.[3] Unprecedented catalytic transformation of robust ethers into secondary alcohol has been achieved using a cobalt pincer catalyst via [1,2]-Wittig rearrangement.[4] The mechanistic studies confirmed the involvement of radical pathway in this transformation. Cobalt pincer catalyzed deoxygenation of aldehydes, ketones, alcohols and ethers to their corresponding alkanes was achieved.[5] Exhaustive reduction of esters to alkanes was reported.[6] Recently, deoxygenative coupling of ethers to alkanes was achieved.[7] These green catalytic transformations will be presented and discussed.



Scheme 1. Cobalt-Pincer Catalyzed Organic Transformations

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IL-3

Dr. Sanjay Kumar Singh
Professor

Department: Department of Chemistry
Institute: Indian Institute of Technology Indore
Address: Simrol, Indore, M.P.
Contact Number: +91-731-660-3350
e-Mail: sksingh@iiti.ac.in

Sanjay Kumar Singh received his MSc (Chemistry) degree in 2002 from A.P.S. University, Rewa, India and his doctoral degree (Chemistry) from the same university (with Prof. D.S. Pandey) in 2007. During his doctoral research, he also worked as a CSIR SRF with Prof. D.S. Pandey at Banaras Hindu University. He worked as a JSPS postdoctoral fellow and AIST postdoctoral scientist with Prof. Q. Xu at AIST, Osaka, Japan (2008-2011) and Alexander von Humboldt (AvH) postdoctoral Fellow with Prof. P.W. Roesky at Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany (2011-2012). In May 2012, he joined as an Assistant Professor in Chemistry at the Indian Institute of Technology (IIT) Indore, India, and since Feb. 2022, he is Professor of Chemistry at IIT Indore. His research is focused on catalyst development for H_2 production, Biomass/waste transformation and CO_2 capture and conversion.

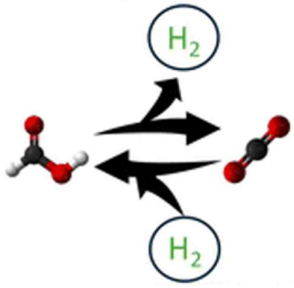
Awards and Professional Recognitions

- Bronze Medal, Society for Materials Chemistry (SMC), India, 2024
- Visiting Professor, ICAT, Hokkaido University, Japan, 2024 and 2026
- Visiting Professor KIT, Germany (AvH Fellowship for Research Stay), 2024
- Dr. S.S. Deshpande National Award, India, 2022
- Associate Dean, International Relations, IIT Indore, 2021-2024
- Award of Excellence in Teaching, IIT Indore, 2017
- Alexander von Humboldt (AvH) Fellowship (1140404), Germany, 2011-2013
- JSPS Postdoctoral Fellowship (P-08615), Japan, 2008-2010
- Editorial Advisory Board member, ACS Sustain. Chem. Eng., 2020
- Editorial Advisory Board member, ChemCatChem, Wiley-VCH, since 2022

Aqueous-phase hydrogenation-dehydrogenation of CO_2-formate couple over ruthenium catalysts

*Sanjay Kumar Singh**
Catalysis Group, Department of Chemistry, Indian Institute of Technology Indore, Simrol, Indore (M.P.), email: sksingh@iiti.ac.in

Abstract:
The intensive usage of fossil fuels and industrial processes causes a rise in the atmospheric CO_2 concentration from 280 ppm (prior to pre-industrial era) to 425 ppm (present), which is a major cause of raising global temperature. This sudden surge accentuates the compelling necessity to embark on mitigating measures to reduce CO_2 emissions, as advocated by the Intergovernmental Panel on Climate Change (IPCC) and the 2015 United Nations Climate Change Conference (COP21) in Paris. To effectively address this critical problem, several carbon capture and utilization (CCU) process for CO_2 capture and the further catalytic valorisation of CO_2 to valuable chemical feedstocks such as formic acid (FA)/formate, methane, alcohols and hydrocarbons, have been extensively explored in recent past both at the laboratory and industrial scales.[1-3] Among them, hydrogenation of CO_2 to FA/formate has gained more attention, as FA can also be used in direct formic acid fuel cell (DFAFC) and it is also a potential hydrogen storage material (4.3 wt% H_2).[2,3] In this regard, we demonstrated enhanced catalytic activity for CO_2 hydrogenation to formate and formate dehydrogenation in water over ruthenium catalysts.[1-5] Such system which can catalyse CO_2 hydrogenation to formate and further dehydrogenate formate through a reversible hydrogenation-dehydrogenation cycles of CO_2/formate couple is an important development for aqueous-phase carbon neutral hydrogen storage and release systems.



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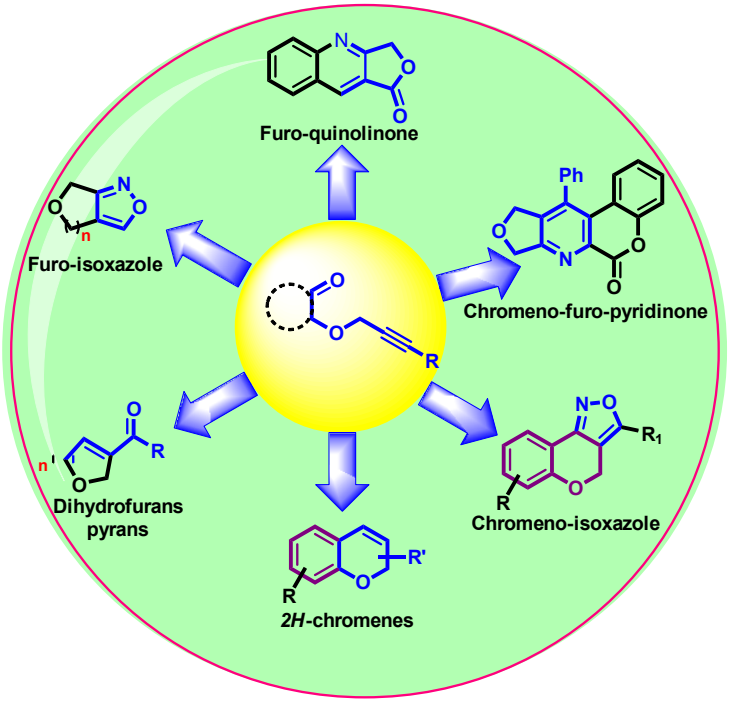
IL-4

Dr. Mahender Khatravath received his B.Sc. and M.Sc. degrees in Organic Chemistry from Osmania University, Hyderabad, India. He obtained his Ph.D. in 2016 from the University of Hyderabad, in association with the Dr. Reddy's Institute of Life Sciences (DRILS), under the supervision of Prof. Prabhat Arya. Following his doctoral studies, he pursued postdoctoral research with Dr. D. Srinivasa Reddy (currently Director, CSIR-IICT) at CSIR-NCL, Pune, for 1.5 years, followed by a seven-month postdoctoral stint with Dr. Ch. Raji Reddy at CSIR-IICT, Hyderabad. In 2018, he joined Transcell Oncologics Pvt. Ltd. as a Research Scientist, where he was actively involved in medicinal chemistry programs aimed at discovering novel leads against challenging and previously undruggable targets, including K-RAS, c-Myc, and Wnt signaling pathways.

In 2019, he joined the Department of Chemistry, Central University of South Bihar, Gaya, India, as an Assistant Professor. His research interests span synthetic organic chemistry, with particular emphasis on the development of novel synthetic methodologies for the construction of biologically privileged scaffolds, total synthesis of natural products, and design of natural product–inspired macrocycles. The Khatravath Research Group also focuses on the synthesis of diverse functionalized heterocyclic frameworks, including quinolines, isoquinolines, tetrahydroquinolines, coumarins, and furans, through innovative domino cyclization, annulation, and cycloaddition strategies involving alkyne activation.

Title: Alkyne-Assisted Cascade Cyclizations/cycloadditions for the Synthesis of Biologically Relevant Nitrogen- and Oxygen-Containing Heterocycles

Abstract: The development of efficient and sustainable strategies for the synthesis of heterocyclic frameworks remains a central objective in modern organic synthesis and medicinal chemistry. This presentation highlights our recent advances in alkyne-assisted cascade reactions for the rapid construction of structurally diverse nitrogen- and oxygen-containing heterocycles, including coumarins, furans, isoxazoles, isoquinolines, quinoline-fused lactones, and furocoumarins. These methodologies exploit the unique reactivity of alkynes through carbonyl–alkyne metathesis, intramolecular nitrile oxide cycloaddition (INOC), and intramolecular Povarov (imino Diels–Alder) cyclization to efficiently assemble complex molecular architectures from readily accessible substrates. The developed protocols exhibit broad substrate scope, excellent functional-group tolerance, operational simplicity, and high atom economy, providing practical and sustainable routes to valuable heterocyclic scaffolds. Furthermore, many of the synthesized frameworks closely resemble structural motifs found in biologically active natural products and pharmaceutical agents, underscoring their potential utility in medicinal chemistry and drug discovery. Overall, this work demonstrates the versatility of alkyne-assisted cascade transformations as powerful synthetic tools for the efficient preparation of medicinally relevant heterocyclic compounds.



IL-5

Dr. Debabrata Maiti

Institute Chair Professor
Department of Chemistry
Indian Institute of Technology Bombay, Mumbai, India

Prof. Debabrata Maiti is an Institute Chair Professor in the Department of Chemistry at IIT Bombay and a leading researcher in the field of catalytic organic synthesis and C–H activation. His research focuses on developing innovative catalytic methodologies that enable efficient and selective functionalization of inert carbon–hydrogen bonds, thereby simplifying the synthesis of complex organic molecules.
Prof. Maiti received his Ph.D. from Johns Hopkins University in 2008 under the supervision of Prof. Kenneth D. Karlin. He subsequently carried out postdoctoral research at Massachusetts Institute of Technology with Prof. Stephen L. Buchwald, where he worked on catalytic reaction development. In 2011, he joined IIT Bombay as a faculty member and established an internationally recognized research program in modern catalytic chemistry.

His group works on several cutting-edge areas of chemical synthesis, including remote C–H functionalization, bioinspired catalysis, heterocyclic chemistry, photocatalysis, and electrochemical catalysis. These approaches aim to create sustainable and efficient strategies for the synthesis of pharmaceuticals, natural products, and advanced functional materials.

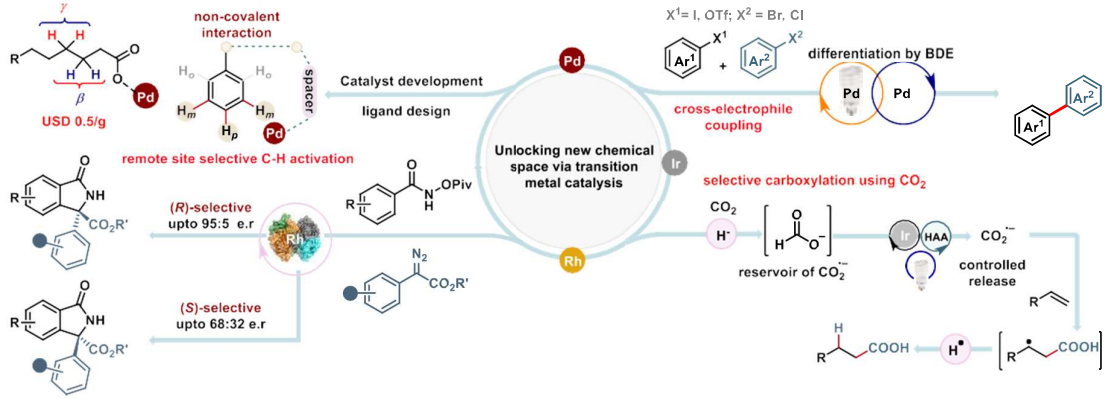
Prof. Maiti's research has contributed significantly to the advancement of site-selective C–H bond activation, enabling the transformation of simple starting materials into complex molecular architectures through fewer synthetic steps. Such strategies have broad applications in medicinal chemistry, agrochemicals, and materials science.

He has received numerous national and international recognitions for his contributions to synthetic chemistry, including election as Fellow of the Royal Society of Chemistry (FRSC) and Fellow of the Indian Academy of Sciences (FASc). Prof. Maiti currently serves as the Editor-in-Chief of the journal Synlett, contributing to the advancement and dissemination of research in synthetic organic chemistry

Unlocking new chemical space via selective catalysis

Debabrata Maiti
Department of Chemistry, IIT Bombay,
www.dmaiti.com, Email : dmaiti@iitb.ac.in

The limitations of traditional cross-coupling methods—including the need for prefunctionalized coupling partners, substrate instability, and high synthetic cost—continue to restrict access to new chemical space and molecular complexity. To address these challenges, our research focuses on the development of direct C–H functionalization and cross-electrophile coupling (XEC) strategies. Selective functionalization of remote C–H bonds remains particularly challenging because these sites are often inaccessible for the formation of energetically favorable organometallic pre-transition states. In particular, linear-chain aliphatic frameworks containing non-distinguishable methylene units often exhibit flat reactivity profiles, making site-selective C–H activation exceptionally difficult. To overcome this challenge, we have devised distinct methodologies for the activation of C–H bonds at different positions along aliphatic chains. Through rational ligand design, we are able to achieve regioselective activation of specific C–H bonds. We hypothesized that positioning the reactive metal catalyst in close proximity to a targeted remote C–H bond could overcome these limitations. Accordingly, we developed covalently attached template-directed approaches that rely on precise spatial arrangement of the directing group to achieve selective activation of remote C–H bonds. More recently, we demonstrated that non-covalent interactions can similarly control catalyst–substrate orientation, enabling highly selective C–H activation. In parallel, we are exploring cross-electrophile coupling as a powerful platform for constructing unsymmetrical (hetero)biaryls from abundant and stable (hetero)aryl electrophiles. We have developed a ligand-controlled, visible-light-driven monometallic XEC methodology that enables direct coupling of (hetero)aryl halides and pseudohalides. Additionally, our laboratory is pursuing new paradigms for the utilization of small molecules such as CO_2 and SO_2 as sustainable feedstocks. Through renewable visible-light photocatalysis, we aim to transform these abundant molecules into a broad range of valuable chemicals and materials.



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IL-6

Dr. Srinivasan ANANDAN
Scientist-F

Department: Centre for Advanced Materials & Batteries
Institute: International Advanced Research centre for Powder Metallurgy & new Materials (ARCI)
Address: Balapur P.O. Hyderabad-500005
Contact Number: 9989677949
e-Mail: anandan@arci.res.in

Dr. Srinivasan Anandan is a Senior Scientist with extensive research experience in energy-storage materials and advanced nanomaterials, with expertise in Li-ion and sodium-ion batteries, supercapacitors, and Li-ion capacitors. His research focuses on the development, scale-up, characterization, and cell-level validation of electrode materials, including carbon-coated $LiFePO_4$ (LFP), LFMP, LTO, high-voltage cathodes, hard carbon, and advanced porous carbons. His expertise spans kg-scale material production, electrode fabrication, cylindrical and pouch-cell development, and battery-module validation for electric vehicle and storage applications.

He has contributed to major national R&D programmes on advanced batteries through various sponsored and industrial projects and is currently a Principal Investigator in the ANRF MAHA-EV Mission. His research has resulted in 80 publications with more than 5,300 citations and 28 patent filings (20 international and 8 Indian). He has played a key role in the technology development and transfer of indigenous battery materials. The battery-grade LFP production technology, for which he is the Lead Inventor, has been transferred to M/s ALTMIN Pvt. Ltd., Hyderabad, with global exclusive rights outside India and non-exclusive rights in India, and to M/s Allox Minerals Pvt. Ltd., Hyderabad, with non-exclusive rights in India. As an Associate Inventor, he also contributed to the successful transfer and commercialization of self-cleaning photocatalytic material technology to M/s Resil Chemicals Pvt. Ltd., Bengaluru, which was subsequently introduced into the textile market.

His major recognitions include the ECSI–Amar Raja National Award 2024, Young Scientist Award from the Materials Research Society of Japan (IUMRS-ICA 2008), prestigious JSPS Fellowship, and recognition among the Top 2% Scientists worldwide in Materials Science by Stanford University in 2020 and 2022. He was selected as an Associate Fellow of the Telangana Academy of Sciences (2019) and participated in the LEADS 2024 Programme jointly organized by INSA and the National Centre for Good Governance.

He currently serves as a Research Advisory Board Member at MLR Institute of Technology, Hyderabad, and as a BIS Member of the Electrotechnology in Mobility Sectional Committee (ETD 51). His work integrates fundamental research, technology translation, scale-up, industrial collaboration, and commercialization of indigenous energy-storage technologies supporting India's advanced-battery and electric-mobility ecosystem.

Indigenous Electrode Materials for Li- and Na-Ion Batteries: Advancing from Fundamental Science to Technology Translation

Srinivasan Anandan

Centre for Advanced Materials & Batteries, International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI), Balapur, Hyderabad, Telangana, India.

Email: anandan@arci.res.in

Translational research is critical for converting laboratory-scale materials innovations into scalable, high-performance, and commercially viable technologies for strategic energy-storage applications. This presentation highlights ARCI's integrated efforts in the development, scale-up, electrochemical validation, and technology transfer of indigenous electrode materials for lithium-ion batteries (LIBs) and sodium-ion batteries (NIBs).

For LIBs, ARCI has developed a cost-effective high-energy milling route for the synthesis of in-situ carbon-modified $LiFePO_4$ (C-LFP), enabling scalable production with controlled composition and enhanced electronic conductivity. The technology has been demonstrated at the 15–20 kg batch scale and validated at the cell level, followed by patenting [1] and technology transfer to M/s Allox Minerals and M/s ALTMIN Pvt Ltd.,. A 300 kg/day pilot-scale C-LFP production facility has subsequently been established by ALTMIN at the ARCI incubator, demonstrating a clear pathway from material development to industrial scale-up.

For NIBs, ARCI has developed $Na_3V_2(PO_4)_3$ (NVP), a NASICON-type cathode, using high-energy milling [2] followed by controlled calcination. The material delivers a specific capacity of 110–115 mAh g^{-1} with >80% capacity retention after 200 cycles. The synthesis has subsequently been scaled up to 20 kg per batch, and pouch-cell fabrication is currently in progress. ARCI has also developed $Na_4Fe_3(PO_4)_2P_2O_7$ (NFPP), an Fe-based polyanionic cathode, exhibiting a specific capacity of 112 mAh g^{-1} at 0.1C and 60 mAh g^{-1} even at 100C, highlighting its excellent high-rate capability and structural robustness. In parallel, sustainable hard-carbon anodes derived from bio- and industrial-waste feedstocks have been developed, delivering a specific capacity of 309 mAh g^{-1} at 20 mA g^{-1} with >80% capacity retention after 100 cycles [3].

Overall, the work demonstrates ARCI's end-to-end approach to indigenous battery-material development, spanning fundamental materials engineering, scalable synthesis, electrochemical performance evaluation, cell-level validation, pilot-scale production, and technology transfer. These efforts contribute toward establishing a robust domestic ecosystem for advanced Li- and Na-ion battery manufacturing. Further insights into materials design, structure–property–performance relationships, scale-up challenges, and commercialization strategies will be discussed during the presentation.

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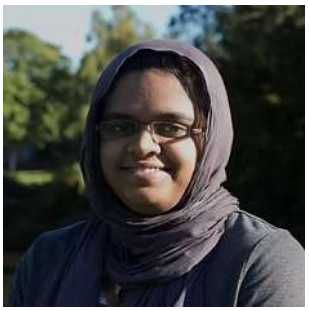
IL-7

Dr. Rositha Kuniyil
Associate Professor

Department: Chemistry
Institute: IIT Palakkad
Address: B03-127, Sahyadri Campus, IIT Palakkad
Kanjikode West, Palakkad – 678623, Kerala, India
Contact Number: 04923 209 1056
e-Mail: rosithak@iitpkd.ac.in



Education and Professional Experience

2013 - MSc chemistry from Indian Institute of Technology Bombay (IITB), Mumbai, India
2017 - PhD in theoretical and computational chemistry from ICIQ (Institut Català d'Investigació Química), Tarragona, Spain
2018-2020 Postdoctoral Researcher at the Georg-August Universität Göttingen
2020-2021 Postdoctoral Researcher at the University of Pittsburgh, USA
2021- 2025 Assistant Professor – IIT Palakkad
August 2025 onwards - Associate Professor – IIT Palakkad

Awards and Recognitions:

Thieme Chemistry Journals Award 2026
Kerala Government Yuva Pratibha Puraskar (Science) 2021

Research area – Computational chemistry

- Small Molecule Activation
- Insilico Catalyst Design
- Design of Artificial Metalloenzymes
- Photocatalysis
- Catalysis with 2D-Materials

Transition State Model for the Manganese Based Chemical Hydrogen Battery

Rositha Kuniyil*
Department of Chemistry, IIT Palakkad, rosithak@iitpkd.ac.in

Abstract: Transition state modeling is a powerful tool for unraveling the mechanistic intricacies of chemical reactions. It plays a pivotal role in the design of new catalytic systems, facilitating progress in the field of catalysis.[1] A carbon-neutral chemical hydrogen battery is the most sustainable approach for the storage and transportation of the hydrogen fuel.[2] Herein, with the aid of transition state models, we decipher the mode of activity of the pincer-ligated manganese complex towards achieving the reversible hydrogenation and dehydrogenation process for the efficient H_2 storage and release (Figure 1).[3] We identified the critical contributions from the basic amino acids specifically lysine and potassium lysinate as well as the influence of solvent, counterions, and water in the reaction. In addition, we have probed into the role of non-covalent interactions during the capture and release of CO_2 with potassium lysinate, which enabled to achieve the carbon-neutral hydrogen battery system.[4]

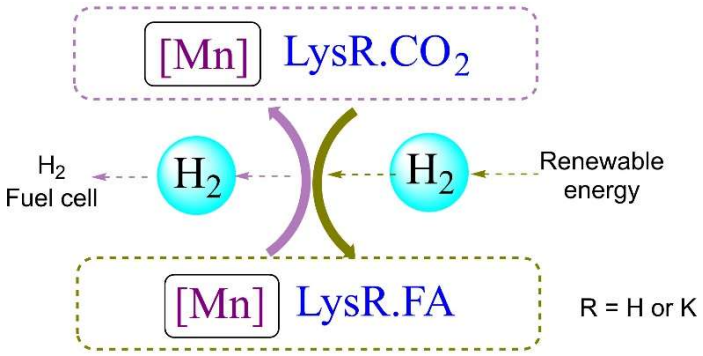


Figure 1: Reversible hydrogenation (of CO_2) and dehydrogenation (of formic acid) in presence of a manganese pincer complex with lysine (LysH)/potassium lysinate (LysK)

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Dr. Akkattu T. Biju
Professor

Department of Organic Chemistry
Indian Institute of Science, Bangalore
Bangalore, 560012, Karnataka.
Ph: +91-80-2293-2646
E-mail: atbiju@iisc.ac.in
Homepage: https://atbiju.in/

Associate Editor, *Synthesis*
Advisory Board, *Chem. Commun.*
Advisory Board, *Org. Chem. Front.*
Advisory Board, *SynLett.*
International Advisory Board, *Asian J. Org. Chem*.
Editorial Board, *Green Synth. Catal.*
Editor-in-Chief, *J. Heterocyclic Chem*. (2019-2024)

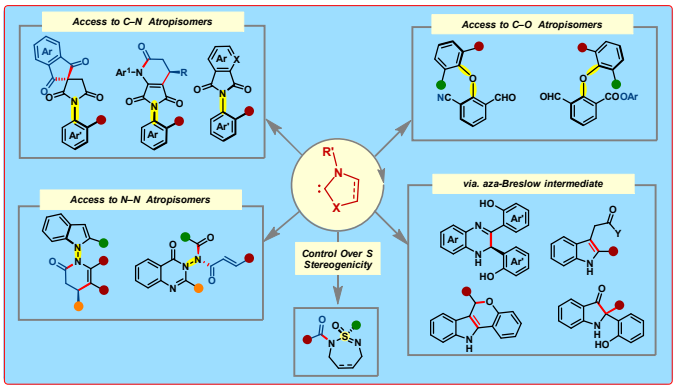
A. T. Biju received his M. Sc. from Sacred Heart College Thevara (affiliated to MG University, Kerala, India) and Ph.D. under the guidance of late Dr. Vijay Nair at the CSIR-NIIST (Formerly RRL), Trivandrum, India. Subsequently, he has been a post-doctoral fellow with Prof. Tien-Yau Luh at the National Taiwan University, Taipei and an Alexander von Humboldt fellow with Prof. Frank Glorius at the Westfälische Wilhelms-Universität Münster, Germany. In June 2011, he began his independent research career at the CSIR-National Chemical Laboratory, Pune. In June 2017, he moved to the Department of Organic Chemistry, Indian Institute of Science, Bangalore, where he is a professor presently. His research focuses on developing strategies using N-heterocyclic carbene (NHC) organocatalysis, and strain-release driven reactions of arynes, donor–acceptor cyclopropanes and bicyclobutanes.

N-Heterocyclic Carbene-Catalyzed Synthesis of C-N, C-O and N-N Axially Chiral Molecules

Akkattu T. Biju

Department of Organic Chemistry, Indian Institute of Science, Bangalore-560012, India
Email: atbiju@iisc.ac.in

Organocatalysis using N-heterocyclic carbene (NHCs) has been widely utilized for the polarity reversal of aldehydes (*umpolung*).[1] Although NHC catalysis is well demonstrated for the enantioselective synthesis of target molecules, related application to the synthesis of axially chiral molecules is limited (especially the heteroatom-containing axis). We have recently reported the NHC-catalyzed atroposelective synthesis of C-N axially chiral N-aryl succinimides,[2] phthalimides/maleimides,[3] N-N axially chiral 3-amino quinazolinones,[4] indoles and pyrroles as well as C-O axially chiral diarylethers.[5] In addition, precise control over S(VI)-stereogenic center has recently be achieved by the enantioselective synthesis of N-acyl cyclic sulfonimidamides.[6] The details of these works will be discussed.



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Dr. N. Lakshminarasimhan
Scientist-G
Department: Electro-organic & Materials Electrochemistry Division
Institute: CSIR-Central Electrochemical Research Institute (CECRI)
Address: Karaikudi 630 003, Tamil Nadu, India
Contact Number: +91-4565-241503
e-Mail: laks.cecri@csir.res.in / nlnsimha@gmail.com

Dr. N. Lakshminarasimhan is Scientist-G working at Electro-organic and Materials Electrochemistry Division, CSIR-Central Electrochemical Research Institute, Karaikudi. He also holds the responsibility as the Head, Director's Technical Cell and Head, Central Instrumentation Facility. He is a Fulbright Scholar and Professor, Academy of Scientific and Innovative Research (AcSIR), Ghaziabad. His broad research area is solid state chemistry and materials science, and his work focuses on functional materials for energy and environmental applications. He research work involved in understanding structure-morphology-property relationships in photofunctional materials including phosphors, photocatalysts, and dye-sensitized solar cells, electroceramics and energy materials. He studied at Muthurangam Govt. Arts College, Vellore, and obtained his undergraduate and postgraduate degrees in Chemistry from University of Madras. He obtained his PhD from Indian Institute of Technology (IIT) Madras, Chennai in 2005. Further, he carried out his postdoctoral research work at Pohang University of Science and Technology (POSTECH), South Korea before joining CSIR-CECRI in 2009. He has **63 publications** in international peer-reviewed journals and his **H-index is 26**. He is a recipient of **'CSIR Young Scientist Award in Chemical Sciences for 2012'** which is first-of-its-kind in the history of CSIR-CECRI. He was a **Fulbright Visiting Scholar** and a Courtesy Faculty at Department of Chemistry, Oregon State University, USA during April-December, 2021. Dr. N. Lakshminarasimhan is an **Editorial Board Member of the journal Solid State Sciences, Elsevier**. He is an elected **Member of International Centre for Diffraction Data (ICDD), USA**. He is an active member of American Chemical Society, American Association for the Advancement of Sciences, Electrochemical Society USA, and life member of Materials Research Society of India, Chemical Research Society of India, Luminescence Society of India, Magnetics Society of India, and Society for Advancement of Electrochemical Science and Technology.

Interface and Interphase in Functional Materials

N. Lakshminarasimhan* [a, b]

[a]*Electro-organic & Materials Electrochemistry Division*
CSIR-Central Electrochemical Research Institute, Karaikudi 630 003, Tamil Nadu, India.
[b]*Academy of Scientific & Innovative Research, Ghaziabad, 201 002.*
E-mail: laks.cecri@csir.res.in

Abstract: Functional materials are those which exhibit specific functionalities or properties such as dielectric, electronic, magnetic, optical, etc. The functionality of materials can originate from the bulk structure and/or from the surface. These leverages tuning the properties of functional materials through modifications either in the bulk, such as compositional tuning or at the surface. In inorganic-organic hybrid materials, the organic capping ligand, oleic acid, modifies the photofunctional properties of red-emitting inorganic phosphors through the surface interactions at the inorganic-organic interface, resulting in white-light emission [1-3]. Similarly, in the case of inorganic-inorganic oxide nanocomposites, the properties can be tuned depending on the nature of the individual component oxides, and their interactions at the interphase and at grain boundary interface, which alter the electroceramic properties (dielectric and proton conduction) and energy storage characteristics [4-6]. Thus, understanding the interface and interphase is essential for tuning the properties of functional materials.

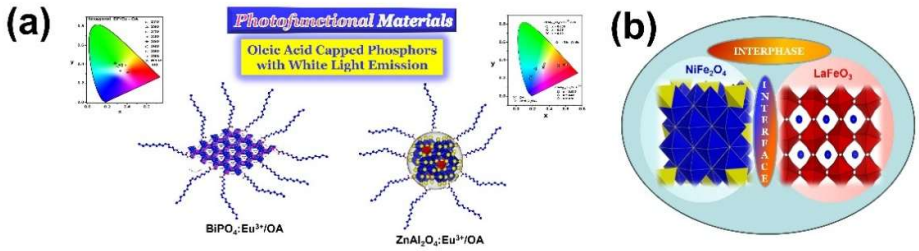

Figure. Schematic representation of (a) oleic acid anchored phosphors, and (b) interface & interphase in spinel-perovskite $NiFe_2O_4$-$LaFeO_3$ nanocomposite.

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IL-10

Dr. Devarajulu Sureshkumar
Associate Professor
Department of Chemical Sciences
IISER Kolkata
Contact Number: 7384542702
e-mail: suresh@iiserkol.ac.in
Homepage: http://www.iiserkol.ac.in/~suresh/

Career Profile:

Devarajulu Sureshkumar completed his B. Sc. in Chemistry and M. Sc. in Organic Chemistry at the University of Madras. He earned his Ph.D. in 2007 under the supervision of Prof. S. Chandrasekaran in the Department of Organic Chemistry at IISc Bangalore. From 2008 to 2010, he was an AvH postdoctoral fellow, working with Dr. Martin Klussman in Prof. Benjamin List's group at the Max-Planck-Institut für Kohlenforschung in Germany. He then undertook a short postdoctoral associate position with Prof. Wilhelm Boland at the Max-Planck Institute for Chemical Ecology in Jena, Germany, before moving to Japan as a JSPS fellow. There, he worked with Prof. Masakatsu Shibasaki at the Institute of Microbial Chemistry in Tokyo (2010-2015). He joined the IISER Kolkata as a faculty member in the Department of Chemical Sciences in February 2015. His research focuses on visible-light-mediated photocatalysis, fluorination, and C(sp^3)–H functionalization.

Significant Awards/Achievements:

Early Carrier Research Award-2017 from SERB, Government of India.
Ramanujan Fellowship-2016 from SERB/DST, Government of India.
JSPS Fellowship-201 for Foreign Researchers (Pathway to University Positions in Japan).
JSPS Fellowship-2011 at the Institute of Microbial Chemistry, Tokyo, Japan.
AvH Fellowship-2008 at Max-Planck Institute for Khölenforschung, Germany.

Representative Publications:

1. Photocatalytic remote C(sp^3)–H alkylation of long-chain alkenes: A tandem multicomponent approach via radical translocation. Ghosh, K. G.; Das, D.; Srinivasu, V.; Pal, K.; **Sureshkumar, D***. *Chem. Sci.* **2026**, *17*, 5888-5898.
2. EDA-Complex-Enabled Remote 1,n-Difunctionalization of Alkenes via Distal C(sp3)–H Activation. Srinivasu, V.; Bagchi, S.; Ghosh, K. G.; Giri, S.; Sureshkumar, D.* *Org. Lett*. **2026**, *28*, 5764-5768.
3. Dual Strain-Release Cascade for Accessing sp3-Rich Azetidine-BCP Frameworks Bearing Multiple Quaternary Carbon Centers. Srinivasu, V.; Balaraju, A.; Kumar, N. A. K.; Sureshkumar, D.* *Org. Lett*. **2026**, *28*, 3856-3861.
4. Open-Air Organophotocatalysed Ring-Closing Cascade Trifluoromethylation of Dienes Inside Supramolecular Gel. †Singh, S.; †Pal, K.; Mal, S.; **Sureshkumar, D***. **Haldar, D***. *J. Org. Chem.* **2026**, *91*, 3633-3640. († equal contribution)
5. Strategic Installation of the -CH_2CF_3 Motif *via* Transition-metal-catalyzed C–H Functionalization. Garai, S.; Sureshkumar, D.* *Chem. Commun*. **2026**, *62*, 10011-10021.

Reaching Remote C(sp³)–H Bonds with Visible Light

Vinjamuri Srinivasu, Shirshendu Giri, **Devarajulu Sureshkumar***
Department of Chemical Sciences, IISER Kolkata, Mohanpur, West Bengal
e-mail: suresh@iiserkol.ac.in

Abstract:
A mild, redox-neutral, and transition-metal-free strategy has been discussed for the tandem perfluoroalkylation and remote C(sp³)–H alkylation of terminal alkenes via organophotocatalysis. The protocol exhibits excellent chemo- and regioselectivity, enabling precise difunctionalization of unactivated alkenes at diverse positions, including 1,10, 1,14, 1,11, 1,7, and 1,6. A key highlight is the unprecedented radical translocation between secondary C(sp³)-centers with comparable bond dissociation energies, marking a significant advance in radical-based synthesis.

Furthermore, a tandem cascade sequence involving trifluoromethylation, 5-exo-trig cyclization, 1,5-radical translocation, and C(sp³)–H alkylation of 1,6-dialkenes has been realized. This multi-component, transition-metal-free approach provides efficient access to highly substituted cyclopentane derivatives. The scalability of the protocol, along with the facile diversification of the products into a range of functional groups, highlights its broad synthetic utility and versatility.

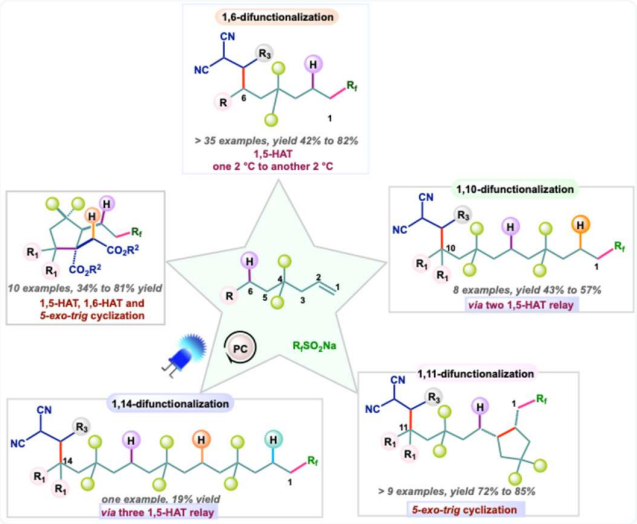

Figure 1. Distal 1,n-difunctionalization of long-chain unactivated alkenes

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IL-11

Mr./Ms./Dr. Sivakumar Shanmugam
Designation: Associate Professor
Department: Organic Chemistry/School of Chemistry Institute: Madurai Kamaraj University, Madurai Address: Palkalai Nagar, Madurai 625 021
Contact Number: 9715452858
e-Mail: shivazzen@mkuniversity.org

Associate Professor: Department of Organic Chemistry, School of Chemistry, Madurai Kamaraj University, Madurai-625 021. (2020 - Present); Assistant Professor: Department of Organic Chemistry, School of Chemistry, Madurai Kamaraj University, Madurai-625 021. (From March 24, 2010 - 2020) Research/Training/Education: UGC-Raman Post-Doctoral Fellow: Division of Translational Imaging, New York State Psychiatric Institute, Columbia University, USA. (Oct. 2013 – 14); Visiting Fellow: (Chemical Biology), Department of Chemistry, Ben-Gurion University of Negev, Israel. (May 2010-June 2010) Post-Doctoral Fellow: Chemical Biology Lab at the Department of Chemistry, Ben-Gurion University of Negev, Israel. (May 2008-March 2010) ; Ph.D. (Organic Chemistry): Department of Chemistry, Pondicherry University, Pondicherry. Guide: Prof. H. Surya Prakash Rao (June 2002-April 2008) Project Fellow, (Organic Chemistry), Industrial Project, Department of Chemistry, Pondicherry University, Pondicherry. Guide: Prof. H. Surya Prakash Rao (Dec 2002-June 2003). Awards/Honours: CRSI Bronze Medal Announced for the year of 2027. By Invitation – Attended National Organic Symposium Trust (NOST)-Organic Chemistry Conference (OCC), 2023 & 2026. Cover Page published in Journal of Materials Chemistry C 2025. Cover page Published in New Journal of Chemistry, 2023, 2025 (2). Convener, CRSI Local Chapter, Madurai (2023-2026). Indo-US UGC-Raman Postdoctoral Fellowship. (2013-2014). DST Young Scientist (FAST TRACK). (2010). By Invitation – Attended Junior - National Organic Symposium Trust (J-NOST)-Organic Chemistry Conference (OCC), 2006. Awarded CSIR-SRF (Senior Research Fellow in Council of Scientific and Industrial Research (CSIR)). 2006. Qualified UGC-CSIR-NET 2001 (Council of Scientific and Industrial Research (CSIR). Qualified GATE ("Graduate Aptitude Test in Engineering") (2000 & 2003). Best Poster Presentation Award at CRSI Local Chapter, Madurai – 625021 (2003).

- Projects Completed: 5 (SERB, DST, UGC, RUSA and TANSCHE)fund genereated ~5.0 Crore
- **Ph.D., Awarded: 11; Ongoing: 06; M.Phil**. Project guided: 13,; M.Sc., : 40. Ongoing: 05; Guided SRF from Indian Academics of Sciences, Bangalore: **20.**
- Paper presented in Conference/Workshop/Seminars: **International: 25; National: 46**
- Publications More than **52** International Journals (JOC's, JMC-C, JPC C, ***ACS Applied Nano Materials***, NJC, Tetrahedron, Tetrahedron Letters, ***ChemPhotoChem, ChemPlusChem,*** **Chemical Biology and Drug Design, Langmuir, ACS Omega, Sensors & Diagnostics etc.,**

Professional Memberships:

- Life Member, Indian Society for Radiation and Photochemical Sciences (ISRAPS)
- Member, American Chemical Society, USA (2014 –2019)
- Life Member, Chemical Research Society of India (CRSI), Bangalore (2011 – Present)
- Life Member - Fluorescence Society of India
- Area of Specialization: Synthetic Organic Chemistry. Field of Interest: Organic Synthesis, AIE. Organo-Boron Chemistry, Organic materials, Sensors.

Title: π-Conjugated Self-Assembled Systems for SDS Detection

Dr. Sivakumar Shanmugam*
Deparment of Organic Chemistry, School of Chemistry, MKU, Madurai-625021.TN

Abstract: The widespread industrial use of Sodium dodecyl sulfate (SDS) in personal care and textile manufacturing has led to increased environmental concerns, necessitating efficient detection strategies. This work introduces a simplified sensing approach using π-conjugated quaternary ammonium compounds (QACs). By employing (2-(methylthio)indeno[1,2,3-gh]phenanthridin-1-yl)(phenyl)methanone and an aza-thiazole hybrid tetraphenylethylene, we exploit the electrostatic attraction between the cationic nitrogen of the probes and the anionic sulfate group of SDS. These interactions facilitate the self-assembly of the molecular system, offering a highly effective and accessible method for monitoring SDS concentrations in varied biological and industrial applications

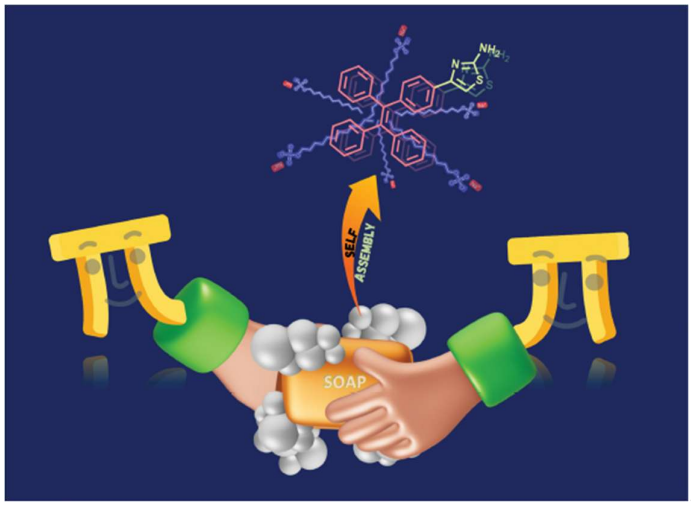

Figure: Plausible sensing mechanism of **TTHI-3** with SDS.

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IL-12

Dr. J. Nithyanandhan
Chief Scientist
Department: Physical and Materials Chemistry Division
Institute: CSIR-National Chemical Laboratory
Address: Dr. Homi Bhabha Road, Pune 411008
Contact Number: 91 20 2590 3050/ 9545280938
e-Mail: j.nithyanandhan.ncl@csir.res.in

Education
2000 – 2006: Ph. D., Organic Chemistry, Indian Institute of Science, Bangalore.
1998 – 2000: Master of Science (Chemistry), Pondicherry University, Puducherry.
1995 – 1998: Bachelor of Science (Chemistry), Ayya Nadar Janaki Ammal College, Sivakasi (Affiliated to Madurai Kamaraj University, Madurai, Tamil Nadu).

Academic research experience
2026 - Present: Chief Scientist, CSIR-National Chemical Laboratory, Pune 411008.
2021- 2026: Senior Principal Scientist, CSIR-National Chemical Laboratory, Pune 411008.
2016- 2021: Principal Scientist, CSIR-National Chemical Laboratory, Pune 411008.
2012- 2016: Senior Scientist, CSIR-National Chemical Laboratory, Pune 411008.
2006 – 2011: Post-Doctoral Associate, University of Miami, Coral Gables, FL, USA.

Research interests
Organic synthesis, Organic photochemistry, Supramolecular chemistry, Photo responsive materials and Dye-sensitized solar cells.

Patents: 3, and Total Publications 64

Selected publications:
1. *Ingole, K. B.; Siby, J.; Pandya, R.; Vanka, K.; Krishnamoorthy, K.; Nithyanandhan, J. Chemistry - An European Journal*, **2026**, *12*, *e70455*.
2. Jadhav, A. P.; Siby, J.; Pandya, R.; Vanka, K.; Krishnamoorthy, K.; Nithyanandhan, J. *ACS Appl. Energy Mater.*, **2025**, *8*, 15459–15470.
3. Ingole, K. B.; Deshmukh, S.; Tushar, V.; Krishnamurty, S.; Krishnamoorthy, K.; Nithyanandhan, J. *ACS Appl. Energy Mater.,* **2024**, *7*, 7982 – 7991.
4. Singh, A. K.; Kavungathodi, M. F. K.; Mozer, A. J.; Krishnamoorthy**,** K.; Nithyanandhan, J. *Langmuir* **2022**, *38*, 14808–14818.
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Professional membership: Chemical Research Society of India (CRSI), Indian Society for Radiation and Photochemical Sciences (ISRAPS), **Luminescent Organic Materials Consortium of India (LOCI).**

Excitonically Coupled Squaraine Dyes for Photocurrent Generation

J. Nithyanandhan
Chief Scientist
Physical and Materials Chemistry Division
CSIR-National Chemical Laboratory, Pune 411008, MH, India
j.nithyanandhan.ncl@csir.res.in

Abstract: Light absorbing chromophores play a vital role in harvesting solar energy in the third generation photovoltaic technologies. Dye-TiO_2 interface plays a key role in efficient charge separation, dye regeneration and diminished charge recombination processes to enhance the device performance in dye-sensitized solar cells (DSSCs). Hence structurally in-built features for the enhanced charge injection and reduced charge recombination processes are required to integrate to the sensitizers. Further, sensitization of dyes on the anatase 101 facet of TiO_2 facilitates the dye-dye interaction which adds challenges in achieving an efficient photo-anode as aggregated dyes exhibit distinct photophysical properties and broaden the light harvesting property due to the formation of H- and J-aggregates. In the light of this, a set of alkyl group wrapped squaraine dyes indicated the structural requirements for the photocurrent generation from the aggregated dyes (**Figure 1**). Extending the □-conjugation in sensitizers help shifting the absorption in the far-red regions of the solar spectrum by which the HOMO levels of the dyes were altered systematically less positive (*vs* NHE) which hampers the dye-regeneration process. To address this issue, excitonically coupled dye is designed to enhance the light harvesting property by maintaining the HOMO energy level and utilized for the DSSC device fabrication.

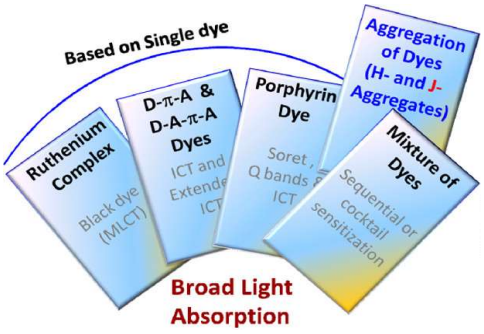

Figure 1: Enhanced light harvesting efficiency of sensitizers by means of aggregation.

References and Notes:

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2. Jadhav, A. P.; Siby, J.; Pandya, R.; Vanka, K.; Krishnamoorthy, K.; Nithyanandhan, J. *ACS Appl. Energy Mater.*, 2025, *8*, 15459–15470.
3. Jadhav, A. P.; Singh, A. K.; Shivankar, B. R.; Siby, J.; Krishnamurty, S.; Krishnamoorthy, K.; Nithyanandhan, J. *ACS Appl. Energy Mater.*, 2025, *8*, 5017 – 5030.

IL-13

Dr. C. M. Nagaraja
Designation: Professor

Department: Chemistry
Institute: Indian Institute of Technology Ropar
Address: Rupnagar, Punjab
Contact Number: 8427545877
e-Mail: cmnraja@iitrpr.ac.in

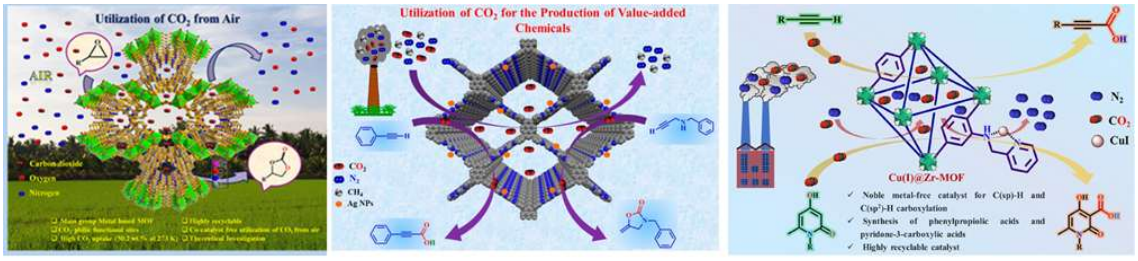
Dr. Nagaraja is a professor of chemistry at the Indian Institute of Technology (IIT) Ropar. He earned his MS degree from Bangalore University and PhD from the Indian Institute of Science, Bangalore. Thereafter, he carried out postdoctoral research at Brandeis University, USA, and Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore. He has been awarded the Japan Society for the Promotion of Science (JSPS) invitational fellowship, the Chemical Research Society of India (CRSI) Bronze Medal, and the Faculty Research Award from IIT Ropar. His research group mainly works on the design of multifunctional framework (MOF/COF) materials for the utilization of carbon dioxide and the generation of solar fuels.

Strategic Design of Framework Materials for Chemical Fixation of Carbon Dioxide into Value-Added Chemicals

Dr. C. M. Nagaraja

Professor, Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar-140001, Punjab, India. E-mail: cmnraja@iitrpr.ac.in

Abstract: The escalating carbon dioxide content in the atmosphere has led to pervasive consequences such as global warming, variations in climate, and erratic weather conditions. To address these detrimental environmental issues, it is imperative to attenuate atmospheric carbon dioxide concentration through selective capture and subsequent storage/utilization. Consequently, carbon capture and utilization (CCU) as a C1 feedstock to generate value-added chemicals and fuels offers dual advantages of mitigating the rising CO_2 concentrations and sustainable generation of high-value compounds/fuels.[1] Especially, selective carbon capture and utilization from direct air has attracted tremendous attention due to its practical applications.[2] In this direction, our research group is working on the rational design of functional framework (MOF/COF) materials incorporated with a high density of CO_2-philic and catalytic sites suitable for simultaneous capture and conversion of carbon dioxide into high-value chemicals under mild conditions.[3-5] Highlights of ongoing research on the strategic design, synthesis, and catalytic investigation of framework materials for the chemical fixation of CO_2 into various value-added chemicals will be presented.



References and Notes:

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Short Invited Lecture - SIL

SIL-1

Dr. Kamini Mishra
Assistant Professor

Department: Chemistry
Institute: Vellore Institute of Technology (VIT), Vellore
Address: Vellore Campus, Katpadi, Vellore, Tamil Nadu
Contact Number: +91 8861539735
e-Mail: kamini.mishra@vit.ac.in

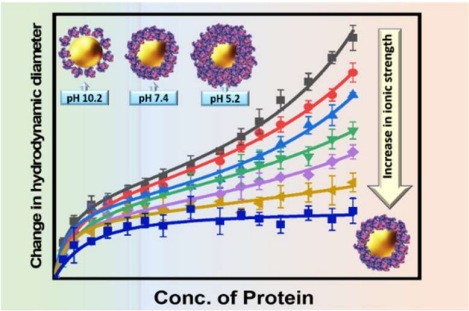
Dr. Kamini Mishra is currently an Assistant Professor in the Department of Chemistry, School of Advanced Sciences (SAS), VIT University, Vellore, where she has been serving since 2019. She received her Ph.D. in Physical Chemistry from the Indian Institute of Science (IISc), Bangalore, India. Her doctoral research focused on protein adsorption at nanoparticle surfaces probed by using second-harmonic light scattering. Her research interests include biophysical chemistry, physicochemical interactions at the nano-bio interface, light scattering techniques, nonlinear optical spectroscopy, and crystal nucleation.

She has published several research articles in reputed international journals, including Physical Chemistry Chemical Physics, The Journal of Physical Chemistry B, Chemical Communications, and Langmuir.

From Monolayer to Multilayer: Electrostatic Control of Protein Adsorption on Gold Nanoparticles

*Kamini Mishra**
Department of Chemistry, School of Advanced Sciences (SAS), VIT University, Vellore
Email: kamini.mishra@vit.ac.in

Abstract: The protein adsorbed on the surface of nanoparticles upon exposure to biological fluids resulting in formation of protein corona that dictates their biodistribution, cellular uptake, and clearance,[1] yet the transition between monolayer and multilayer corona architectures remains poorly resolved due to reliance on *ex situ* separation methods that perturb adsorption equilibria.[2] Here, we use *in situ* dynamic light scattering (DLS) to directly track changes in hydrodynamic diameter upon protein adsorption.[3] The adsorption of three proteins with isoelectric points spanning the acidic, near-neutral, and basic ranges, namely bovine serum albumin (BSA, pI ≈ 4.8), myoglobin (Myo, pI ≈ 7.2), and papain (Pap, pI ≈ 8.72) was investigated onto citrate-capped gold nanoparticles (GNPs) of size 15, 30 and 60 nm as a function of pH (5.2, 7.4, and 10.2) and ionic strength. At pH 5.2, the electrostatic attraction between the negatively charged nanoparticle surface and the positively charged proteins is strongest, all three proteins exhibit multilayer adsorption well described by a Brunauer–Emmett–Teller (BET) isotherm, resulting first-layer and subsequent-layer binding free energies of $\Delta G°_1 \approx -49.5$ to -53.7 kJ/mol and $\Delta G°_2 \approx -41.9$ to -44.8 kJ/mol, respectively. At pH 7.4 and 10.2, adsorption saturates at monolayer coverage fitted with modified Langmuir model, resulting $\Delta G° \approx -52.6$ to -60.6 kJ/mol. Salt-titration experiments at pH 5.2 show that increasing ionic strength progressively screens interprotein electrostatic interaction and drives reversion to monolayer adsorption, allowing to delineate the contributions of electrostatic and non-electrostatic forces in multilayer protein adsorption. This salt-induced regression directly confirms that multilayer formation arises primarily from protein–protein electrostatic interactions at pH 5.2. These results establish pH- and salt-tuneable electrostatics, rather than protein concentration alone, as a controllable switch for corona architecture.



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3. Mishra, A.; Mishra, K.; Bose, D.; Chakrabarti, A.; Das, P. K. *Phys. Chem. Chem. Phys.* **2021**, *23*, 24365–24376.

SIL-2

Dr. Sathishkumar Pannerselvam
Assistant Professor
Chemistry, School of Advanced Sciences
Vellore Institute of Technology, Vellore - 14
Contact Number: +91-9003538748
e-Mail: sathishkumar.p@vit.ac.in

Dr. Sathishkumar Panneerselvam began his research in nanomaterials and photocatalysis in the year 2007 and he earned his Ph.D. from the National Institute of Technology (NIT), Tiruchirappalli, India in 2010 and later pursued post-doctoral research at the University of Concepción, Chile. With over 15 years of experience in sonochemistry, photocatalysis and nanomaterials, he has published more than 70 original research articles, ten book chapters and edited two books in Springer nature and IOP publications. He has held various research positions in the international level. After joining Vellore Institute of Technology (VIT), Vellore, India as an Assistant Professor, he has led the Ultrasonics and Advanced Photochemistry Laboratory since 2020.

Sonophotocatalysis – A powerful tool for the destruction of environmental contaminants

*Panneerselvam Sathishkumamr **
Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore – 632014, India
Sathishkumar.p@vit.ac.in

Abstract: Current wastewater treatment technologies fall short, with projections indicating that up to 4.8 billion people may face health issues due to inadequate water purification by 2030. Preventing environmental problems is more effective than addressing their consequences. Hybrid advanced oxidation processes (h-AOPs), such as sonophotocatalysis, offer a sustainable and efficient method for catalytic conversion, decomposing environmental toxins in water without secondary pollution. Recently, MXene-based nanocatalysts have attracted attention due to their unique properties, including high surface area, excellent adsorption capabilities, and internal electric fields, making them ideal for AOP-related applications. Comprehensively discussion to the synergistic benefits of sonophotocatalysis for the degradation of various organic pollutants, sustainable synthesis routes for MXene and its precursor (MAX) and their alignment with SDG targets. Finally, future perspectives on MXene-based nanoarchitectures, synergistic ultrasonic approaches and greener approaches to minimize secondary pollution are outlined to support effective AOP-assisted wastewater treatment.

SIL-3

Dr. Saikat Dutta
Professor

Electrochemical Energy & Sensor Research Laboratory& Advanced Battery Research Laboratory
Amity Institute of Click Chemistry Research & Studies
Amity University
Noida (Delhi NCR), India
E-mail: sdutta2@amity.edu

Saikat Dutta is a professor of chemistry at Amity University Uttar Pradesh (AUUP) Noida. He is a Fellow of the Royal Society of Chemistry, UK. Prof. Dutta's research focuses on advanced interfacial electrochemistry, advanced metal and metal-ion batteries, atomic-scale single- and multi-atom materials, capacitors, and sensors. Prof. Dutta has been at Amity University for the last eight years, and during this phase, he has established two advanced research laboratories, "Electrochemical Energy & Sensor Research Lab" and "Advanced Battery Research Lab" in AICCRS with the funding and equipment grant support of DBT, ANRF, and DST. In the past, Prof. Dutta was a Senior Researcher at the US DOE Catalysis Centre for Energy Innovation at the Department of Chemical and Biomolecular Engineering, University of Delaware, USA. Prof. Dutta is also editorial advisory and editorial board member of several Wiley, ACS, and RSC journals.

Atomic Interface in Electrodes of Na-Ion Batteries and Electrochemical Mimicking of Enzymes

Diffusion kinetics of Na^+ in a sodium-ion battery coin cell drastically restrain the rate capability and capacitance of the anode. We have found that reversible conversion and diffusion of Na^+ in our anode material, consisting of Fe-N_4-O_2 sites closely coupled with Fe_3C clusters, establish strong electronic interactions and optimize tuning of their composition ratios in a WNC. DFT simulation of Na^+ migration energy (eV) along the diffusion path exhibits a significant discharge-specific capacity of 318 mA hg^{-1} at a current density of 50 mAg^{-1}.[1] The electrochemical analysis supports the role of Fe─N bonding in modulating the electronic environment of Na^+ diffusion sites. The incorporation of Fe─N_4─O_2 in WNC results in 1) faster Na^+ diffusion through hollow (H) sites, 2) stretching of the Fe─N bond during discharge cycles. In addition, Fe─N_4─O_2–WNC anode promises the manufacturing of advanced SIBs from a renewable material and thereby enhances the investigation of sodiophilic Fe─N sites.

Ni–N_4–PAN–NC, consisting of an atomic Ni–N_4 site, mimics the intramolecular electron-harnessing of natural laccase (LAC) confined in a zeolitic imidazolate framework-8 (LAC@ZIF-8) for anodic electrooxidation of bisphenol-A (BPA). We have introduced a facile π-conjugated unit of polyacrylonitrile (PAN)-resorcinol-derived N-doped conjugated -C≡N. The atomically dispersed Ni single atom in Ni–N_4-PAN–NC exhibits high activity for the paired electrolysis of ORR and the electrooxidation of BPA with an enhanced current density. An increased power density with increased concentration of BPA in the absence of ABTS suggests a DET mechanism of BPA electrooxidation on Ni–N_4, unlike a MET in the presence of ABTS when using LAC@ZIF-8. Thus, single-atom Ni−N_4 opens avenues for a DET mechanism.[2] Therefore, in this talk, I will be speaking about our recent reports on a sodium-ion battery coin cell used for investigating diffusion kinetics and Na^+ diffusion features. Further, I will speak about the enhanced power density in biofuel cells by using isolated-atom-containing single-atom and dual-atom electrodes, wherein their electronic features are suitable for electrochemical process design, especially biofuel cells.

SIL-4

Dr. Suresh Babu Kalidindi
Associate Professor

Department: Chemistry
Institute: Central tribal university of Andhra Pradesh
Address: Vizianagaram
Contact Number: 8747877361
e-Mail: suresh.babu@ctuap.ac.in

Dr. Suresh Babu Kalidindi obtained his PhD from the Indian Institute of Science (IISc), Bangalore, in 2010. Following his doctoral studies, he conducted postdoctoral research as an Alexander Humboldt fellow at Ruhr University, Germany, and later worked at the University of Liverpool as post-doc fellow. Upon returning to India, Dr. Suresh joined the Poornaprajna Institute of Scientific Research (PPISR), Bangalore, as a DST-INSPIRE faculty member. He subsequently served as a UGC-Assistant Professor at Andhra University before assuming his current role as Associate Professor at the Central Tribal University of Andhra Pradesh.

Currently, Dr. Suresh and his research group focus on the hybridization of nanomaterials with porous framework materials, integrating reticular chemistry with nanoscience. This approach aims to develop new functional advanced materials with applications in clean energy, gas sensing, and nanocatalysis.

Advanced Materials for Hydrogen Sensing under Oxygen-Deprived Conditions

Suresh Babu Kalidindi* and Ganesh Korada, Valle Krishnaveni
Department of Chemistry, Central Tribal University of Andhra Pradesh (CTUAP), Kondakarakam, Vizianagaram, Andhra Pradesh, 535 003, India, Email: suresh.babu@ctuap.ac.in

Abstract: Hydrogen is a clean, zero-emission energy carrier with immense potential to replace carbon-based fuels in the global transition toward sustainable energy. However, its high diffusivity and wide flammability range demand efficient and reliable hydrogen sensors to ensure safety in production, storage, and utilization. Among various sensing technologies, chemiresistive sensors are particularly attractive due to their simplicity, fast response, miniaturization capability, and cost-effectiveness.[1-4] Conventional semiconducting metal oxides (SMOs -based chemiresistive sensors typically operate through oxygen-assisted surface reactions, in which adsorbed oxygen species act as the primary reactive sites for H_2 detection. Consequently, their sensing performance is strongly dependent on the presence of oxygen, making them less effective under oxygen-deprived or inert conditions.

However, reliable H_2 monitoring in inert atmospheres is critical for several technologically important applications, including the safety of fast nuclear reactors, semiconductor manufacturing, and hydrogen fuel-cell systems. In fast reactors, argon (Ar) is used as a cover gas over liquid sodium, where H_2 generated from sodium–moisture reactions can serve as an indicator of coolant leakage. Similarly, inert atmospheres are employed during semiconductor processing and in hydrogen storage, transportation, and fuel-cell systems to minimize contamination and prevent the formation of explosive H_2–air mixtures. Despite these requirements, efficient H_2 sensors capable of operating rapidly and reliably in oxygen-deprived environments remain scarce. This talk will highlight our recent efforts toward developing advanced semiconductor oxide–metal–organic framework (MOF) hybrid materials for H_2 sensing under inert conditions. Particular emphasis will be placed on materials design, interfacial interactions, sensing mechanisms, and strategies for achieving rapid response and recovery at room temperature. These developments provide new opportunities for next-generation H_2 sensors for safety-critical applications where conventional oxygen-dependent sensing mechanisms are ineffective.

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SIL-5

Dr. Ramaraj Ayyappan
Assistant Professor

Department: School of Chemistry
Institute: IISER-TVM
Address: Vithura-695551
Contact Number: 9741965388
e-Mail: ramaraj.ayyappan@iisertvm.ac.in

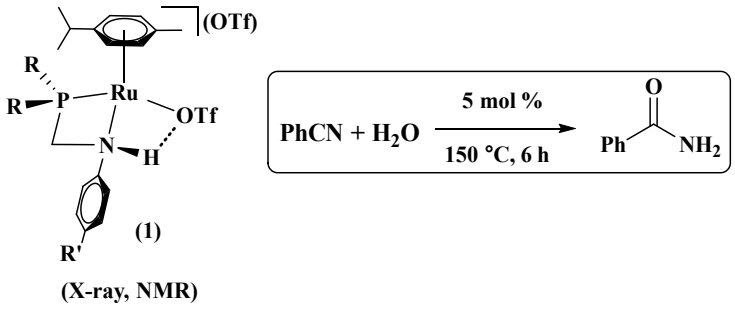
I was born and raised in Nilakottai, Tamilnadu, India. I have completed PhD in the area of small molecules activation working under the guidance of Prof. Balaji R Jagirdar, IISc, Bangalore. Subsequently gained further experience and exposure in the two post-doctoral stays one at the historical LCC-CNRS, Toulouse and the second at University of South Wales, SERC centre, Pontypridd. Since Aug 23, 2022, I am working as a assistant professor at IISER-TVM, Thiruvananthapuram, Kerala, India. My research work focuses on the development of tailored transition-metal complexes for challenging chemical transformations towards sustainability.

Tunable *α*-aminophosphine-Ligated cationic Ru-Cymene Complexes for the Hydration of PhCN

Dr. Ramaraj Ayyappan and Deepthy Devassy, Alex Andrews*
School of Chemistry, IISER-TVM, Thiruvananthapuram, Vithura-695551, Kerala, India.
ramaraj.ayyappan@iisertvm.ac.in

Abstract: Catalytic hydration of nitrile is a useful reaction to produce very important amide functional groups. This route would be atom economical and green transformation over conventional methods which involves harsh conditions, poor functional group tolerance and generate waste by products. However, this reaction requires dual activation of C≡N triple bond of nitriles (RCN) and H_2O. Largely, two bond activation pathways are prevalent for RCN (a) direct coordination with metal (M–CNR) (b) metal-ligand cooperative strategy (MLC). Whereas pendant nitrogen functionalized ligands (L–N) are designed for the co-activation of H_2O via hydrogen bonding.

Based on this understanding, a series of moderately air-stable cationic ruthenium-triflate [Ru(η^6-cymene)(k^2-R'$_2$*P*-(CH_2)NH-R)(OTf)]OTf complexes supported by α-aminophosphine ligands (α-P,N) were isolated in very good yields and thoroughly characterized including NMR, IR spectroscopy and Sc-XRD. These complexes can be tuned easily by modifying R-group on the phosphorus and the *p*-R' of N-phenyl of α-P,N ligand. Especially, the later modification becomes crucial in controlling the hemilability of nitrogen. Indeed, these complexes were found to be good catalysts for the PhCN hydration into benzamide (scheme 1) performing on par with the literature reported example[1] using 5 mol % of **1**, 150 °C, 6 h. Preliminary mechanistic details will also be disclosed.



Scheme 1: Hydration of PhCN using cationic ruthenium-cymene-phosphino-amine complexes (**1**).

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SIL-6

Dr. Akshai Kumar
Associate Professor

Department: Chemistry
Institute: Indian Institute of Technology Guwahati
Address: Guwahati – 781039, Assam, India.
Contact Number: +91-8133036890
e-Mail: akshaikumar@iitg.ac.in

Akshai Kumar is a M.Sc. in inorganic chemistry from Mangalore University and a PhD in Coordination and Organometallic Chemistry from Indian Institute of Science, Bangalore, After Post-doctoral stints in Goethe University, Frankfurt, Germany, and at Rutgers, The State University of New Jersey, New Brunswick, US in 2015, he was appointed as Assistant Professor in Chemistry at the Indian Institute of Technology Guwahati.

He has about 21 years of experience in the area of organometallic chemistry, inorganic chemistry, homogeneous catalysis, and heterogenization of molecular catalysts. He has authored 65 research articles in peer-reviewed journals, including one in Chemical Reviews (Impact Factor = 54.301), in addition to 6 book chapters, 4 US patents (granted), 2 INDIAN patent (granted), 3 US patents (filed), and 5 INDIAN patents (filed). He has extensive experience in utilizing organometallic compounds for homogeneous and heterogeneous catalysis.

With a particular emphasis on base metals, the research group of Dr. Akshai Kumar investigates the pincer-base-metal chemistry and their role in catalyzing C-H activation/functionalization mediated C-C bond formation of alcohols via radical/organometallic pathways that ultimately lead to synthesis of green hydrogen, high value fuels and specialty chemicals starting from waste under thermo- and electrochemical conditions. This includes conversion of unproductive hydrocarbons to fuel-grade chemicals, upgrading low-energy density ethanol to high-energy density fuels and generation of green hydrogen via transformation of inexpensive glycerol, ethanol and methanol to high value lactic acid, acetic acid and formic acid respectively. Currently, research on development of novel catalytic system towards generation of green hydrogen from water is underway. Attempts are also being pursued to develop powerful catalytic systems under photochemical and/or electrochemical conditions to fabricate Direct Alcohol fuel-cell (DAFC) stacks containing non-noble, environmentally benign electrode assemblies built using state-of-art technologies capable of meeting futuristic low-power and high-power energy demands.

He is a member of Indian Young Academy of Science, Member of Bureau of Indian Standards, and fellow of the Indian Chemical Society. He is a Core member of CO2 India Network: Society for CO_2 Research and Innovation (SCRI) https://www.co2india.org/ From January 2025, he is a PAC member, Prime Minister's Early Career Research Grant and National Post-Doctoral Fellowship, Anusandhan National Research Foundation, New Delhi. He is also a chairperson of the Special Evaluation Committee of NIRAMAYA (Northeast Incubator for Rapid Acceleration of Medical and Allied Innovations) Program under AAHII & BioNEST Incubator. Currently, in addition to Associate Professor in Chemistry, he is the Head, Centre for Nanotechnology at IIT Guwahati.

Pincer-Metal Complexes in Thermo-Catalysis & Electro-Catalysis for Generation of Hydrogen, Fuel and Specialty Chemicals

Akshai Kumar*
Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati – 781039, Assam, India

Abstract: Current global research is greatly focused on the development of greener, sustainable and atom-economical methods for production of hydrogen, versatile fuels and value-added chemicals from readily available natural resources such as biomass apart from water. While organometallic catalysts have offered immense promise towards hydrogen production via electrochemical splitting of water,[1] they have also enjoyed great success in dehydrogenative transformation of alcohols for the generation of hydrogen, fuels and specialty chemicals.[2] For efficient catalysis, it would be desirable to have a subtle balance between catalyst stability and reactivity.[3] For nearly five decades now, it has been more often found, that pincer-metal complexes perform exceedingly well in striking this balance.[3]

With a particular emphasis on base metals, the current talk would provide a glimpse on the pincer chemistry that is being investigated in our lab, while shedding light on their role in catalyzing C-H activation/functionalization mediated C-C bond formation of alcohols via radical/organometallic pathways that ultimately lead to synthesis of hydrogen, high value fuels and specialty chemicals.[4] The talk would also delve into our recent attempts towards electro-reforming of not only feed-agnostic alcohols to value-added products[5] but also environmentally viable water to hydrogen.

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SIL-7

Dr. Amit Ashok Vernekar
Senior Scientist

Department: Inorganic and Physical Chemistry Laboratory
Institute: CSIR-Central Leather Research Institute
Address: Chennai, Tamil Nadu, India
Contact Number: 8861102787
e-Mail: amitvernekar.clri@csir.res.in

Dr. Amit A. Vernekar completed his undergraduate and postgraduate studies at Goa University and earned his Ph.D. in 2015 from IISc-Bangalore under the guidance of Prof. G. Mugesh. He then secured a prestigious postdoctoral associateship at MIT (2015-2018), working with renowned bioinorganic chemist Prof. Stephen J. Lippard. Currently, he serves as a Senior Scientist at CSIR-CLRI, Chennai.

Dr. Vernekar has authored numerous impactful research papers, many published in esteemed journals such as Nature Communications, JACS, Angewandte Chemie, and Chemical Science. His research focuses on functional nanomaterials, bioinorganic and biomimetic chemistry, nanocatalysis, and hydrogen storage and generation. He has made significant contributions to the development of nanozyme technology.

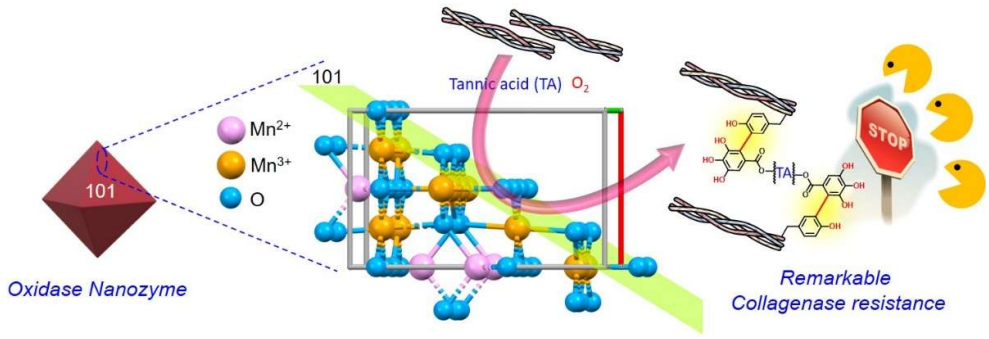
His accolades include the Gandhian Young Technological Award (GYTI) in 2015, the ASDF Best Scientific Researcher award in 2016 (Michigan, USA), the Prof. Soundararajan Medal, and the Best Ph.D. Thesis award from IISc-Bangalore. Dr. Vernekar was also a finalist among the top 45 young scientists globally for the prestigious Reaxys Ph.D. Prize in 2015 in Hong Kong and received the CSIR Young Scientist Award in Chemical Sciences in 2021. He is also a selected member of the INSA-Indian National Young Academy of Science (INYAS).

Beyond Small-Molecule Substrates: Expanding the Catalytic Horizons of Nanozymes for Transforming Biomaterials

Amit Ashok Vernekar
CSIR-Central Leather Research Institute (CLRI), Chennai 600020, India

Abstract: Nanozymes, a class of artificial enzymes, have attracted significant attention in recent years. Following the discovery of intrinsic peroxidase mimetic activity of magnetic nanoparticles in 2007, there has been a surge in the development of various nanozymes that mimic enzymes such as peroxidases, oxidases, hydrolases, and certain antioxidant metalloenzymes. However, the advancement of nanozymes faces several challenges, including compromised selectivity, specificity, and efficiency, as well as low biocompatibility and difficulties functioning within cellular environments.

We have been working on addressing challenges of artificial enzymes. In this presentation, I will present our recent efforts to enhance the catalytic capabilities of an oxidase nanozyme in activating the major structural protein, collagen, for covalent crosslinking. This innovative biomaterial demonstrates 100% resistance to protease attacks, significantly expanding the substrate repertoire of nanozymes beyond small molecules. Our work merges nanozymes' chemistry to produce collagen biomaterials with remarkable enzymatic stability, highlighting the way for new applications in biomedicine and materials science.



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SIL-8

Dr. Susanta Kumar Bhunia
Associate Professor

Department: Department of Chemistry
Institute: Vellore Institute of Technology
Address: School of Advanced Sciences, VIT, Vellore
Contact Number: 9800067154
e-Mail: susanta.bhunia@vit.ac.in

Biographic details:

Dr. Susanta Kumar Bhunia received B.Sc. and M.Sc. degree from Vidyasagar University, West Bengal. He got awarded PhD in 2015 from Indian Association for the Cultivation of Science, Kolkata. He worked on tunable fluorescent carbon dots synthesis, functionalization for biomedical and environmental applications during his PhD tenure. Then he moved to Ben Gurion University of the Negev, Israel for his post-doctoral study. Next, he did his second post-doctoral study at Technion – Israel Institute of Technology, Israel. Then he joined as Assistant Professor in Vellore Institute of Technology, Vellore campus in December 2018. Currently he is working as Associate Professor in the same institute. He has published 50 articles so far in different renowned peer-reviewed journals including ACS, Nature, RSC, Wiley, Elsevier.

Research interests:
1. Synthesis of fluorescent and non-fluorescent nanomaterials
2. Surface functionalization
3. Colorless pollutants selective detection and their effective removal
4. Light emitting diode
5. Degradation of microplastics

Selective and Ultrasensitive Detection of Hypochlorite and Glutathione using Chiral and Bright Green Fluorescent MXene Quantum Dots

Susanta Kumar Bhunia[*,1], Santanu Bera[1], Evangeline Lawrence[2], Kamalesh S[2], Vijay Sithaiyan[1], Umarfaruk S. Sayyad[3], Somen Mondal[3], Anbalagan Moorthy[2]*

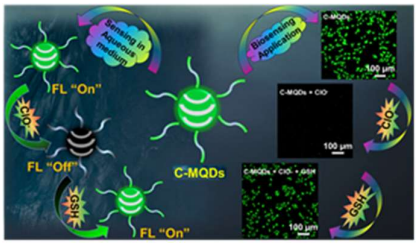
[1]*Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India*

[2]*Department of Integrative Biology, School of Biosciences and Technology, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India*

[3]*Institute of Chemical Technology, Mumbai Marathwada Campus Jalna, Jalna, Maharashtra, 431203, India*

**Corresponding author email address: susanta.bhunia@vit.ac.in*

Abstract: MXene quantum dots (MQDs) exhibit excellent optical properties and good biocompatibility, making them promising materials for sensing and biomedical applications. We report the synthesis of bright green emissive chiral MQDs (CMQDs) with the highest fluorescence quantum yield of 59% by
using a simple solvothermal method. The synthesized C-MQDs exhibited a maximum emission at 495 nm upon excitation at 400 nm. Notably, the fluorescence intensity of the C-MQDs was strongly reduced after the addition of hypochlorite (ClO^-) ions. Mechanistic studies indicated that this quenching occurred through a static quenching process, resulting from the formation of a nonfluorescent complex between ClO^- ions and the surface functional groups of the C-MQDs. Surprisingly, the fluorescence
was restored after the addition of glutathione (GSH) to the C-MQDs-ClO^- complex, as GSH reduced the ClO^- ions. As a result, the fluorescence "on/off/on" behavior of the C-MQDs was used to detect ClO^- and GSH with very good limit of detection (LOD) as 33 and 50 nM, respectively. Furthermore, the analytes were successfully detected inside living cells, demonstrating the probe's capability for intracellular sensing applications. Moreover, ClO^- ions were detected in real water samples with a very good recovery, even in the presence of other contaminants. These results demonstrate that such a nanoprobe has great potential in therapeutic applications.



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Oral Presentation- OP

OP-1

Optoelectronics and electron-beam-induced phase transformation studies on CdS-Ag_2S alloys/ superlattices

Jyotsna Chaturvedi*[1], *Balaji R. Jagirdar*[1]

[1] *Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore - 560012, India*

E-mail address: jcchaturvedi@gmail.com

Abstract: CdS/Ag_2S-based structural chemistry has evolved from cation-exchange reactions, where CdS-to-Ag_2S conversion preserved nanoparticle morphology, to the emergence of new crystal phases and heterostructures [1]. Cation and anion exchange strategies have enabled high-entropy alloys and superlattice architectures with enhanced optoelectronic and catalytic properties [2]. CdS-based heterostructures are promising for photochemical water splitting and optoelectronics, although rapid electron-hole recombination limits their performance [3]. Dodecanethiol-capped monoclinic AgCdS alloy nanocrystals exhibit mono-exponential photoluminescence decay and superior electrochemical hydrogen evolution activity in neutral media [4]. In contrast, octadecylamine-capped wurtzite AgCdS alloys show delayed carrier recombination due to ligand-induced surface defects. Octadecylamine-mediated CdS/Ag_2S superlattices display dual-band emission and tunable interfacial optical responses. Under high-energy electron irradiation, ligand-rich AgCdS@PVP (K-30) nanocomposites undergo anisotropic etching, anion-lattice desorption, and AgCd intermetallic formation. In contrast, ligand-deficient AgCdS@PVP promotes phase transformation and lattice-column rearrangement, highlighting ligand-controlled structural evolution under electron-beam exposure.

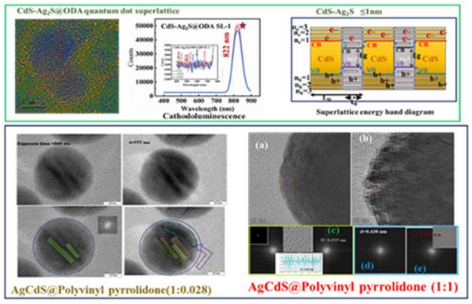

Figure: CdS- Ag_2S superlattice band engineering and e-beam-induced phase transformation in AgCdS nanocrystals

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OP-2

Upgradation of Ethanol to *n*-Butanol Catalysed by Pincer-Iridium Complex

Kamla Devi Netam,[a] *Vikas,*[a] *Andrew S. Weller,**[b] *Akshai Kumar**[a,c]

a. Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati 781039, Asam, India

b. Department of Chemistry, University of York, York YO10 5DD, U.K

c. Center for Nanotechnology, Indian Institute of Technology Guwahati, Guwahati 781039 Assam, India

Email: akshaikumar@iitg.ac.in

Abstract: The growing demand for sustainable liquid fuels has intensified interest in converting renewable bio-ethanol into higher-value bio-butanol, which possesses superior fuel properties and broader industrial applicability.[1,2] In this context, the Guerbet reaction offers an attractive catalytic route for ethanol upgrading through dehydrogenation, C–C coupling, hydrogenation, followed by water elimination step.[3]

In this work, pincer-iridium[4] catalyst was employed for the direct transformation of bio-ethanol to bio-butanol under relatively mild conditions. The study demonstrated that pincer-iridium complex is highly effective for ethanol upgradation, with catalyst structure strongly influencing activity, selectivity, and turnover frequency. Under the optimized reaction conditions, the catalyst delivers significant ethanol conversion and good yield toward *n*-butanol within a short duration. The study employs a minimal catalyst loading with base, that resulted in good yields and selectivity of *n*-butanol surpassing other reported catalyst till date. The catalytic outcomes are thoroughly characterized by gas chromatography analysis qualitatively and quantitatively. Further, the involvement of molecular catalyst was systematically studied by the several control experiments and reaction intermediates were identified by HRMS analysis. Based on the experimental evidences, the plausible mechanism is proposed and complimented through detailed DFT studies. Overall, this work highlights a promising and energy-efficient strategy for valorising bio-ethanol into *n*-butanol using molecular Ir catalyst.

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OP-3

Dual-Mode Near-Infrared (NIR) Chemosensors for Sensing and 3D-printed Device Applications

Avijit Kumar Das, Hazeena Shinziya*
Department of Chemistry, CHRIST (Deemed to be University), Hosur Road, Bangalore, Karnataka 560029, India
Email: avijitkumar.das@christuniversity.in

Abstract:

Multifunctional chemosensors constitute a versatile and powerful class of molecular tools capable of detecting a broad spectrum of targets, ranging from biologically relevant cations, anions, and reactive species to complex biomacromolecules such as DNA, proteins, and enzymes. These systems operate through diverse mechanisms, including chemodosimetric reactions, coordination-based recognition, and specific binding interactions. Our research focuses on designing advanced chemosensors supported by theoretical studies to elucidate receptor–analyte interactions, as well as developing water-soluble NIR fluorescent ligands for selective biomolecular detection through groove binding, intercalation, and end-stacking modes. Furthermore, these sensing capabilities are translated into practical platforms by engineering 3D-printed devices functionalized with fluorescent probes, enabling rapid, sensitive, and cost-effective colorimetric and fluorometric detection. These devices are further enhanced with smartphone-based readout systems to facilitate on-site environmental and analytical applications.

Keywords: Multifunctional; 3D-printing; Dual-mode; Chemosensors; NIR; Device

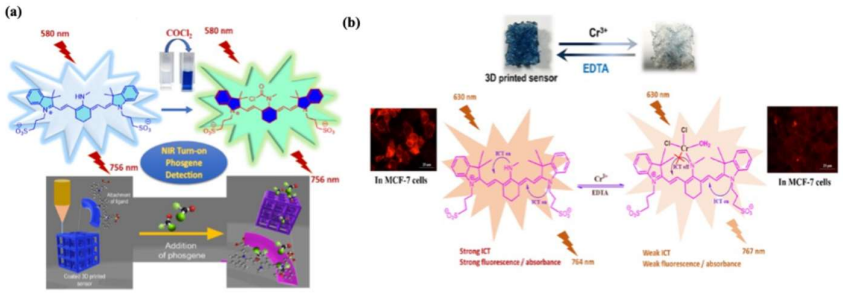

Figure 1: a) 3D-printed detector for rapid Near-IR Turn-on detection of Phosgene. (b) 3D-printed detector for rapid Near-IR Turn-on detection of Chromium.

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OP-4

A general palladium-catalyzed novel class of Hiyama cross-coupling reaction of heteroaryl-substituted coumarinyl conjugates

Sowmiya Carmel Y[a,b], HariPrasad Suresh[b*]

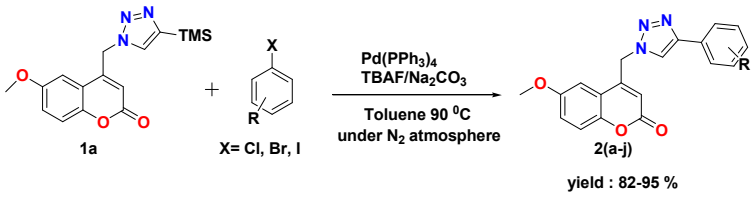
[a]*Department of Chemistry, St. Joseph's Indian Composite PU College, Bangalore-560001, Karnataka, India.* sowmiyacarmel@gmail.com

[b]*Department of Post-Graduate Studies in Chemistry, Central College Campus, Bengaluru City University, Bengaluru - 560001, Karnataka, India.* hariprasad@bub.ernet.in

ABSTRACT

Hiyama cross-coupling is a versatile reaction in synthetic organic chemistry for the construction of carbon–carbon bonds involving the coupling of organosilanes with organic halides using transition metal catalysts in good yields.[1] In recent years, significant progress has been made by researchers toward the synthesis of diversified natural products and pharmaceutical drugs using the Hiyama coupling reaction.[2] This review emphasizes a general palladium-catalyzed Hiyama cross-coupling reaction of heteroaryl conjugates of silylated 6-methoxy-substituted chromen-2-ones with differently substituted aryl halides by employing a catalytic amount of tetrakis(triphenylphosphine)palladium(0) and an excess of tetrabutylammonium fluoride at 90 °C under an N_2 atmosphere. With high chemoselectivity, compounds were formed and isolated in 86-98% yields and characterized spectroscopically using IR, 1H NMR, 13C NMR, MS, and elemental analysis.

GRAPHICAL ABSTRACT



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OP-5

Heteronuclear Correlation Spectroscopy Study of a Few Imidazolium Based Ionic Liquids and Their Silver Complexes

Sainath B. Aher[1], *Prashant N. Muskawar*[2], *Pundlik R. Bhagat*[3]*

[1]*Mahatma Gandhi Vidyamandir's Pharmacy College, Nashik, India 422003, Email: sainathaher88@gmail.com*

[2]*Department of Chemistry, Amlokchand Mahavidyalaya, Yavatmal, India 445002 Email: p.muskawar@gmail.com*

[3]*Department of Chemistry, School of Advanced Sciences, VIT University, Vellore, India 632014 Email: drprbhagat111@gmail.com*

Abstract:

The one-dimensional NMR technique faces a major hurdle in assigning the peaks for the protons associated with particular carbon atoms. Counting and comparing the number of H and C protons in 1D NMR is quite easy, but it becomes tedious while assigning the peaks to particular H and C atoms. The 2D NMR helps in such cases where we have studied the ionic liquids and their silver complexes by the Heteronuclear COSY (HETCOR) technique. The HETCOR technique has helped us to conveniently assign the peaks for compounds containing more than one benzene ring. The HETCOR study revealed the presence of aliphatic and aromatic carbon atoms. One additional thing observed compared to the COSY is the appearance of solvent peaks, such as for DMSO-d_6. Additionally, the slight shifts in NMR values have been comparatively studied for synthesized ionic liquids and their silver complexes. The slight effects of the silver complexation have been thus highlighted in the present study.

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OP-6

Enhanced Bifunctional Electrochemical Activity of Fe doped $NiCo_2O_4$ through Plasma Surface Treatment for toward Overall Water Splitting

Amba Sankar K N*, Ramkrishna Rane, Alphonsa Joseph, Amreen A. Hussain

[1]*Facilitation Centre for Industrial Plasma Technologies (FCIPT), Institute for Plasma Research (IPR), Bhat, Gandhinagar, Gujarat 382428, India*

[2] *Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai 400094, India.*

Email-ambasankarji@gmail.com

Abstract: The development of noble-metal-free bifunctional electrocatalysts is essential for efficient alkaline water electrolysis. In this work, an optimized Fe-doped $NiCo_2O_4$ electrocatalyst was synthesized via a hydrothermal method and subsequently subjected to nitrogen (N_2) plasma surface treatment to enhance its bifunctional performance. The crystal structure, morphology and surface elemental composition were systematically characterized using GI-XRD, SEM and XPS. GI-XRD confirmed the formation of the spinel $NiCo_2O_4$ structure, while XPS revealed plasma-induced electronic structure modulation with increased oxygen vacancies and surface metal defect concentrations. As a result, the plasma-treated Fe-doped $NiCo_2O_4$ exhibited outstanding bifunctional electrocatalytic activity, requiring 320 mV low overpotentials for the oxygen evolution reaction (OER) and 150 mV for the hydrogen evolution reaction (HER) at current density of 50 mA cm^{-2}, together with low Tafel slopes of 79 and 104 mV dec^{-1} respectively. These surface modifications significantly increased the electrochemically active surface area (ECSA) ~ 600 cm^2. In a full cell configuration, the optimized catalyst delivered a lowest onset potential of 1.68 V at 10 mA cm^{-2} and stability conducted up to 300 h in 1.0 M KOH electrolyte. These results demonstrate that nitrogen plasma surface engineering effectively tailors the surface electronic structure of Fe-doped $NiCo_2O_4$ providing an efficient strategy for developing the bifunctional electrocatalysts for overall water splitting.

Keywords: Fe-doped $NiCo_2O_4$, Nitrogen plasma treatment, Surface modification, Bifunctional electrocatalyst.

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OP-7

Bioactive $MnFe_2O_4$ Nanoparticles: Antimicrobial Efficacy and Wound-Healing Assessment

*Radhakrishnan Vidya**

VIT School of Agricultural Innovations and Advanced Learning, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India

**Corresponding author. E-mail: rvidya@vit.ac.in*

Abstract: Manganese ferrite (MnFe2O4) nanoparticles were synthesized via a sol–gel auto-combustion method and characterized for structural, magnetic, and biological properties. XRD confirmed a single-phase cubic spinel structure with a 21 nm crystallite size, while XPS validated Mn^{2+} and Fe^{3+} oxidation states. VSM revealed soft ferrimagnetic behaviour with 22.18 emu/g saturation magnetization. FE-SEM showed a porous morphology (70-75 nm particles), and BET analysis indicated a low surface area of 51.5 m^2/g. No antibacterial activity was observed against tested Gram-positive and Gram-negative strains, while antifungal activity against *Candida albicans* was dose-dependent. Cytotoxicity studies on L929 and Hep3B cell lines confirmed excellent biocompatibility (>75% viability). Notably, scratch wound-healing assays showed 31.26% wound closure at 48 h, compared with 19.65% in controls. These results highlight MnFe2O4 nanoparticles as biocompatible, wound-healing-promoting nanomaterials for biomedical applications.

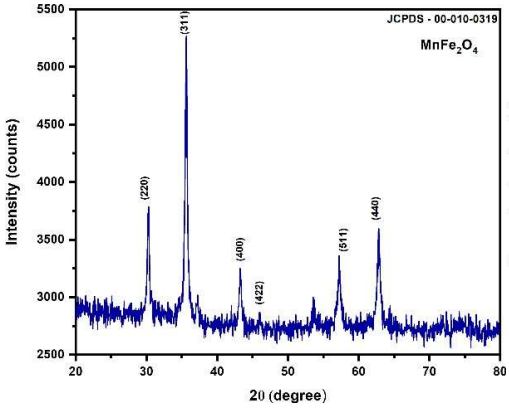

Figure1: Structural analysis of $MnFe_2O_4$ nanoparticles

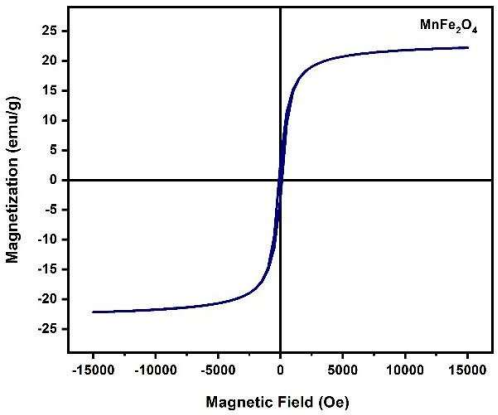

Figure2: M-H curve of $MnFe_2O_4$ nanoparticles

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OP-8

A Versatile Synthetic Pathway to Tunable Persistent Nanophosphors via Deep Eutectic Solvent Mediated Synthesis

Kaleeswarran Periyannan, Zaifa Pan*

National Key Laboratory of Green Chemical Synthesis and Transformation Technology,

College of Chemical Engineering, Zhejiang University of Technology,

Hangzhou 310014, China

kaleeswarran@gmail.com, panzaifa@zjut.edu.cn

Abstract: Persistent Luminescence (PersL) materials are emerging as pioneering probes for in vivo imaging, offering a distinctive advantage over prevailing fluorophores by eliminating the need for constant external excitation. Among Spinel oxides (AB_2O_4) have attracted significant interest for their physicochemical properties, mechanical hardness and high thermal stability. Considering spinel oxides zinc gallate $ZnGa_2O_4$ (ZGO) has distinctly evolved as a research hotspot due to its wide bandgap, intrinsically resilient spinel framework and diverse defects. Within rare earth and transition metal compounds doped Cr^{3+} doped ZGO is specifically appealing because the Cr^{3+} doping ions substitute for octahedrally coordinated Ga^{3+} host cations, producing intense near-infrared (NIR) persistent luminescence around 707 nm[1]. However, conventional synthesis methods frequently struggle to achieve precise control over the defect chemistry, nanoscale morphology and surface properties that are crucial for biological applications. Here, we introduce a simple and an environmentally benign Deep Eutectic Solvents (DES) assisted synthesis of Cr^{3+} doped ZGO using DES as both a reaction medium and a structure-directing agent to produce highly crystalline, uniformly sized spinel oxide nanoparticles (~35 nm) possessing hydrophilic surfaces, eliminating the need for additional ligand exchange. The emission, the centred at ~ 707 nm from the Cr^{3+} $^2E \longrightarrow {}^4A_2$ transition, is particularly well suitable for imaging through biological tissues[2]. Furthermore, the DES environment facilitated, fine defect engineering, reducing oxygen vacancies and antisite defects to serve as optimal charge traps sustaining an NIR afterglow duration exceeding 24 h subsequent to UV or LED excitation. By leveraging the advantages of the DES assisted strategy, we offer a scalable and eco-friendly methodology for designing next-generation PersL materials that can serve as a new class of biomarkers for highly sensitive and specific in vivo optical bioimaging, thereby bridging the gap between advanced material synthesis and clinical translation.

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OP-9

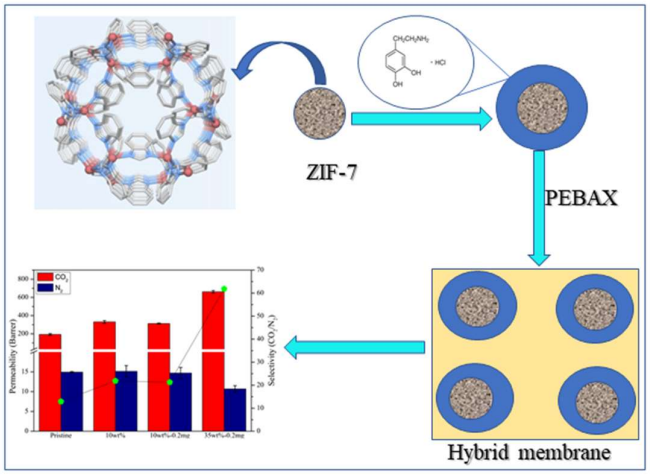
Polydopamine-Modified ZIF-7/Pebax Mixed-Matrix Membranes with Enhanced CO_2/N_2 Separation Performance

Aurobinda Mohanty[1], Han-Jen Ou[1], and Bor Kae Chang[1]*

[1]Department of Chemical and Materials Engineering, National Central University, Taoyuan 320, Taiwan, R.O.C.

E-mail: BKChang@ncu.edu.tw

Abstract: Mixed matrix membranes (MMMs) integrating metal–organic frameworks (MOFs) with polymers are promising for energy-efficient gas separation, yet weak interfacial adhesion between filler and polymer often causes non-selective voids that compromise performance [1]. The aim of this work was to enhance interfacial compatibility and gas separation efficiency by employing polydopamine (PDA) as a bio-inspired interfacial modifier in ZIF-7/Pebax-2533 MMMs. Dopamine, a material small enough to fill voids, inexpensive for mass application, can self-polymerized into polydopamine (PDA) in alkaline conditions. Most importantly, it has great universal and strong adhesion, which is contributed by its benzene ring for π-π stacking and π-cation interactions [2]. The novelty of this study lies in demonstrating that an ultra-low concentration of PDA (0.2 mg mL^{-1}) can effectively eliminate interfacial voids even at high filler loadings (35 wt%), thereby achieving unprecedented performance. The optimized membrane exhibited a CO_2 permeability of 661.8 Barrer and CO_2/N_2 selectivity of 61.85 surpassing the 2019 Robeson upper bound. This work provides a simple, scalable, and low-cost strategy for fabricating high-performance MOF-polymer membranes for sustainable CO_2 capture and gas separation



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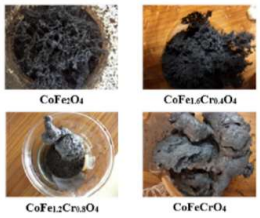
OP-10

Tuning the Structural, Morphological, Surface, and Magnetic Properties of Cr^{3+} substituted $CoFe_2O_4$ ($CoFe_{2-x}Cr_xO_4$) magnetic nanoparticles prepared by self-propagated solution combustion synthesis (CSC) technique

*K. Venkatesan [1], Rajan Babu D [2,] *, Vidya R [3]*
[1] Department of Physics, School of Advanced Sciences and Languages, VIT Bhopal University, Kothrikalan, Sehore, Madhya Pradesh 466 114, India
[2] Department of Physics, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632 014, Tamil Nadu, India
[3] VIT School of Agricultural Innovations and Advanced Learning (VAIAL), Vellore Institute of Technology, Vellore 632 014, Tamil Nadu, India
Corresponding author's email - drajanbabu@vit.ac.in

Abstract: Nowadays, magnetic nanoparticles (MNPs) have played a major role in several applications due to their chemical stability, size and interesting properties. Synthesis of Chromium (Cr^{3+}) ion-substituted $CoFe_2O_4$ ($CoFe_{2-x}Cr_xO_4$) (where x = 0, 0.4, 0.8 and 1.0) magnetic nanoparticles by the solution combustion synthesis (SCS) technique. The structural analysis of the prepared materials was verified by powder X-ray diffraction patterns and Raman analysis. The surface nature and particle size of the prepared materials were found to be 34 ± 5, 18 ± 5, 16 ± 5 and 8 ± 5 nm for the concentrations of x-0, 0.4, 0.8 and 1.0, respectively, which were examined by HR-TEM analysis. The room-temperature measurements based on hysteresis loops confirmed the magnetic transition of Cr^{3+}-substituted cobalt ferrite from ferromagnetic to superparamagnetic nature. The cytotoxicity measurements confirmed the IC_{50} (Inhibiting the 50 % of the cancer cells), and it was found that the prepared magnetic nanoparticles can be used for biomedical applications.

Figure:



As-prepared condition of pure and Cr^{3+}substituted $CoFe_2O_4$ magnetic nanoparticles

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OP-11

Template-based reaction product enumeration software for rapid generation of synthetically accessible compound libraries

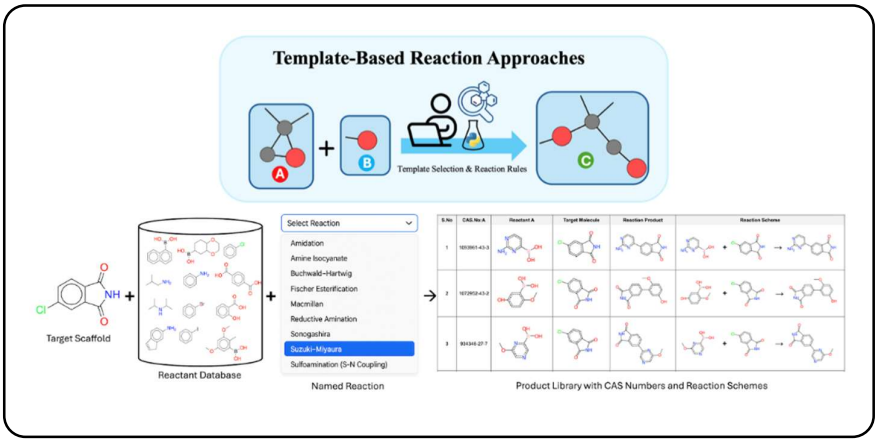
*Sakthivel Balasubramaniyan, Gantzer Philippe, Cooper Simon and Sidorov Pavel**
Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University, Sapporo, Hokkaido, Japan
Email: bala@icredd.hokudai.ac.jp

Abstract: CRePE (Chemical Reaction Product Enumerator) software is a template-based platform developed to accelerate compound-library generation for medicinal chemistry and drug discovery. Conventional analogue design requires chemists to manually identify suitable reactions, search for compatible building blocks, draw individual products, and prepare structure files for synthesis planning and virtual screening. This process is time-consuming, limits chemical-space exploration, and may introduce structural or reaction-related errors.

CRePE automates this workflow by combining a user-provided target scaffold with a reactant database containing CAS numbers and SMILES. Based on transparent, predefined reaction rules, the platform generates synthetically accessible products, complete reaction schemes, and traceable information about the starting materials. The results can be downloaded as SDF, Excel, and HTML files for synthesis planning, molecular docking, ADMET prediction, pharmacophore modelling, and other virtual-screening applications. Basic physicochemical and drug-likeness filters are also included to support compound prioritization.

CRePE currently contains approximately 60 reaction templates covering one-, two-, three-, and four-component reactions. By connecting molecular design with available reactant inventories, CRePE reduces manual effort, minimizes errors, and enables rapid exploration of diverse, synthetically meaningful chemical libraries without relying on black-box artificial intelligence.

Figure/Scheme:



Schematic representation of template-guided reaction product enumeration.

Flash Talk -FT

FT-1

Pincer-Rhodium Catalyzed Conversion of Glycerol to Lactic Acid and Hydrogen

Vikas,[1] *Andrew S. Weller**[2] *and Akshai Kumar**[1,3]
[1]Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati – 781039, India
[2] Department of Chemistry, University of York, York YO10 5DD, UK
[3] Center for Nanotechnology, Indian Institute of Technology Guwahati, Guwahati – 781039, India
Email: akshaikumar@iitg.ac.in

ABSTRACT: The rapid expansion of the biodiesel industry has led to a surplus of glycerol, creating both an environmental challenge and an opportunity for valorization. Transforming waste glycerol into high-value chemicals such as propanediol, dihydroxyacetone, and lactic acid has become a focal point of sustainable catalysis.[1,2] In this work, we present a highly efficient route for the acceptorless dehydrogenation of glycerol to lactic acid, catalyzed by a pincer-rhodium complex. The system achieves up to 94% yield and 98% selectivity towards lactic acid with 90% yield of hydrogen in presence of base, within 36 h. Kinetic investigations reveal a first-order dependence on both catalyst and glycerol concentrations, underscoring their critical roles in the reaction mechanism. Complementary DFT calculations support a metal-centered pathway, identifying σ bond metathesis as the rate-determining step with a calculated barrier ($\Delta G^{\ddagger}_{140}$ = 30.0 kcal/mol), in excellent agreement with experimental barrier ($\Delta G^{\ddagger}_{140}$ = 30.22 kcal/mol) via Eyring equation.

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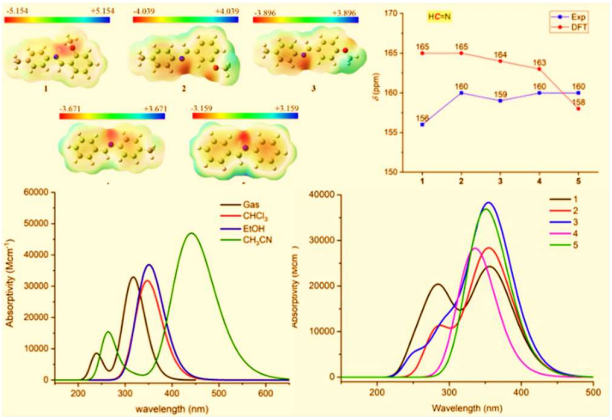
FT-2

Tuning the Spectroscopic, Solvatochromic, and NLO Properties of Diaryl Schiff Bases: Experimental and DFT/TD-DFT Insights

A. Hemamalini,[1] *Carlson Alexander,*[2] *and A. Irudaya Jothi*[1]

[1]*Department of Chemistry, St. Joseph's College, Tiruchirappalli 620002, Tamil Nadu, India.*
[2]*Department of Chemistry, Hong Kong Baptist University, Kowloon Tong, Hong Kong SAR, China.*

Abstract: Diaryl Schiff bases exhibit tunable spectroscopic and nonlinear optical (NLO) properties arising from substituent-induced modulation of molecular polarization and π-electron delocalization within the conjugated framework. Methoxy substitution enhances electron donation through resonance, while its position relative to the imine linkage further influences intramolecular charge transfer, thereby affecting the spectroscopic and NLO properties. In this study, three methoxy-substituted *N*-benzylideneanilines of the type $MeOC_6H_4$–CH=N–C_6H_4–*p*-Me, together with their unsubstituted analogues, were investigated using complementary experimental and computational approaches. Comprehensive spectroscopic, solvatochromic, and DFT/TD-DFT studies were performed to investigate the influence of methoxy substituent position on the electronic structure, ICT characteristics, and optical properties. FT-IR and NMR analyses demonstrate that both the nature and position of the methoxy substituent significantly influence the vibrational frequencies of characteristic IR bands and the shielding/deshielding patterns of proton and carbon nuclei. UV–Vis spectroscopy and TD-DFT calculations reveal bathochromic shifts of the $\pi \rightarrow \pi^*$ transitions with increasing solvent polarity, indicating enhanced intramolecular charge transfer. Molecular electrostatic potential and Mulliken charge analyses show that methoxy substitution on the benzylidene ring promotes resonance donation and π-conjugation, particularly in the ortho and para isomers, resulting in greater molecular polarization and enhanced solvatochromic behaviour. The calculated first hyperpolarizability (β) demonstrates that methoxy substitution strengthens the donor–acceptor interaction, leading to enhanced nonlinear optical (NLO) properties. Overall, positional methoxy substitution provides an effective strategy for tuning the spectroscopic, solvatochromic, and nonlinear optical properties of diaryl Schiff bases, highlighting their potential for photonic and nonlinear optical applications.



Keywords: Diaryl Schiff bases; Methoxy substitution; Positional isomerism; Solvatochromism; DFT/TD-DFT; Nonlinear optical (NLO) properties.

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FT-3

Sunlight Driven Photocatalytic Wastewater Treatment Using a CQD/Ag_3PO_4 Nanocomposite

Aayushi J. Joshi[a], Bibekananda Bhoi[b], Vimlesh Chandra[b]*, *Dheeraj Kumar Singh*[ca]*

[a]*School of Nano Sciences, Central University of Gujarat, Kundhela, Vadodara Gujarat, India, 391107.*

[b]*School of Applied Material Sciences, Central University of Gujarat, Kundhela, Vadodara, Gujarat, India, 391107*

[c]*Department of Physics and Astrophysics, University of Delhi, Delhi-110007, India*

**Corresponding author*

Abstract: In the present work, Carbon Quantum Dot (CQD) integrated silver phosphate (Ag_3PO_4) nanocomposite was synthesized which and evaluated as a solar light driven photocatalyst for the degradation of organic dyes. The successful formation of the nanocomposite was confirmed using various structural, morphological, and optical characterization techniques. Photocatalytic experiments were carried out under natural sunlight, and the degradation of the dye was monitored using UV-Vis spectroscopy. The CQD/Ag_3PO_4 nanocomposite exhibited significantly improved photocatalytic activity compared with pristine Ag_3PO_4, owing to the synergistic interaction between CQDs and Ag_3PO_4. The findings demonstrate the potential of the synthesized nanocomposite as an efficient and sustainable photocatalyst for wastewater treatment applications.

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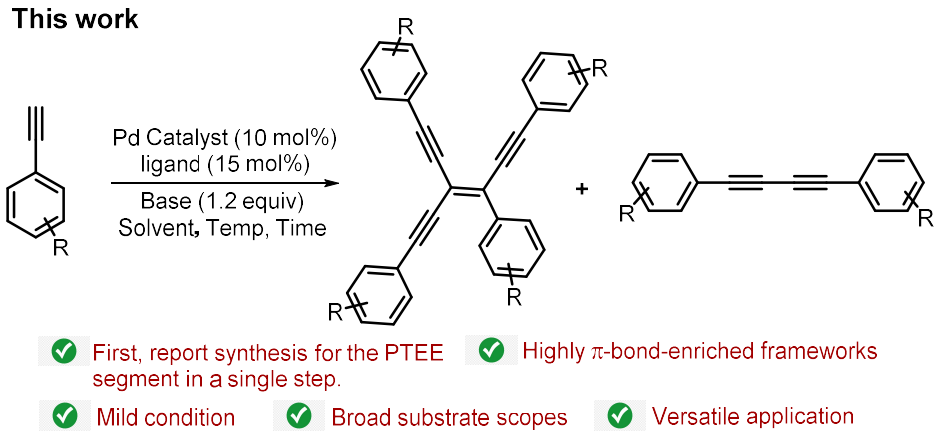
FT-4

Palladium-Catalyzed Iterative Cross-Coupling towards π-Bond-Enriched Phenyltriethynylethylene Frameworks

Manikandan Sekar[1], *Thirumanavelan Gandhi*[1]*
Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu 632014, India.
*E-Mail: velan.g@vit.ac.in, manikandan27799@gmail.com.

Abstract: Transition-metal-catalyzed synthesis of multisubstituted alkenes with highly π-bond-enriched frameworks has attracted considerable attention because of their broad applications in organic materials chemistry, organic semiconductors, biomedicine, and photochemistry. However, the efficient construction of the tetrasubstituted symmetrical phenyltriethynylethylene (PTEE) framework in a single step remains a significant synthetic challenge. PTEE is a phenyl-substituted hybrid of tetraethynylethylene (TEE), a parent π-rich scaffold consisting of an alkene bearing four ethynyl groups, and serves as an attractive platform for enhancing π-bond enrichment in conjugated frameworks. Herein, we report the first single-step synthesis of the PTEE framework from the readily available starting material phenylacetylene through a palladium-catalyzed iterative cross-coupling reaction. This methodology provides access to 23 PTEE derivatives in good yields. All compounds were fully characterized by ^{1}H and ^{13}C NMR spectroscopy, and mechanistic studies were carried out to gain insight into the reaction pathway.



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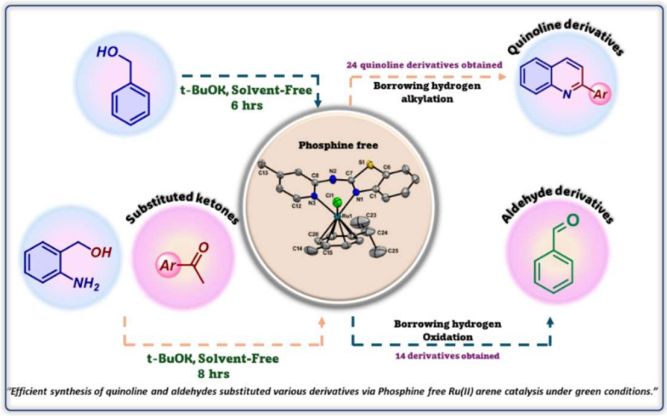
FT-5

Green and Atom-Economic Synthesis of Aldehydes and Quinolines via Solvent-Free Acceptorless Dehydrogenation Catalyzed by Phosphine-Free Ruthenium(II)-arene catalysts

Naveenkumar K and Arup Sinha*

Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, India. Email: arup.sinha@vit.ac.in

Abstract: This study presents the synthesis and characterization of a series of ruthenium(II) arene complexes (C1–C4) derived from phosphine-free, pyridine-based bidentate ligands. The complexes were comprehensively characterized by various spectroscopic techniques, including single-crystal X-ray crystallography, which unambiguously confirmed their molecular structures. Catalytic evaluations demonstrated that these complexes serve as efficient phosphine-free catalysts for the synthesis of aldehydes and quinolines, exhibiting broad functional group tolerance under solvent-free conditions. Spectroscopic investigations under these conditions confirmed the intermediary of a [Ru–H] species, providing mechanistic insight into the catalytic process1,2. The results highlight the potential of these ruthenium arene complexes as sustainable and versatile catalysts for organic transformations3,4. Extensive product formation studies were carried out, providing detailed insights into reaction selectivity, yield optimization, and functional group compatibility



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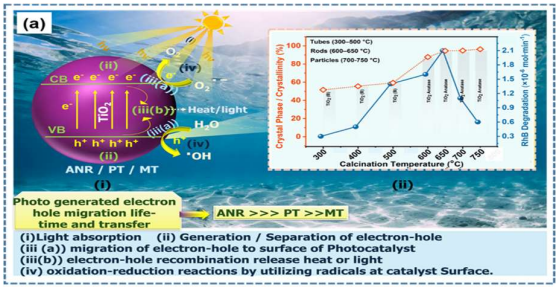
FT-6

$H_2Ti_3O_7$ nanotubes-derived TiO_2 nanorods: Precursor engineering to tailor phase, crystallinity, and photocatalytic performance for efficient dye degradation under natural sunlight irradiation

T.V. Prathima[1,2], N.C. Gangi Reddy[2], M. Mamatha Kumari[1] and M.V. Shankar[1*]
[1]*Nanocatalysis and Solar Fuels Research Laboratory, Department of Materials Science & Nanotechnology, Yogi Vemana University, Kadapa 516005, Andhra Pradesh, India*
[2]*Department of Chemistry, Yogi Vemana University, Kadapa 516005, Andhra Pradesh, India*
*shankarnano@yvu.edu.in

Abstract: This work reports phase, morphology, and crystallinity-tailored anatase TiO_2 nanorods derived from hydrothermally synthesized $H_2Ti_3O_7$ nanotubes. Comprehensive material characterization revealed that the quasi-one-dimensional morphology and superior crystallinity accelerated the photogenerated charge-carrier dynamics, with a 10-fold increase in carrier lifetime (under optimized calcination conditions of 650 °C @ 8 °C·min^{-1} for 4 h) compared to the precursor anatase TiO_2 photocatalyst. This enhanced photocurrent generation, and efficient charge-carrier separation significantly increased the photocatalytic degradation rate of Rhodamine B (RhB) dye under midday peak sunlight irradiation. For the first time, in diurnal sunlight irradiation experiments conducted from morning to evening, the degradation performance of RhB was directly correlated with simultaneous variations in the light spectrum and intensity (comprehensive data table provided). Photocatalytic experiments conducted to optimize essential parameters demonstrated 100% RhB degradation at pH 11 within 30 min, owing to favorable material characteristics: charge-carrier dynamics, reactive oxygen species generation, and subsequent catalytic redox reactions. Stability tests confirmed the reusability of the catalyst over multiple cycles without significant loss of activity. This work highlights the beneficial roles of the anatase phase, nanorod morphology, and high crystallinity in harvesting abundant sunlight for environmental remediation and a sustainable future.



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FT-7

Blue LED-driven synthesis of benzoyl-guanidine hybrids *via* radical–radical cross-coupling

*Krishnarao Jayaram Desai, Annamalai Pratheepkumar**
Catalysis and Fine Chemicals Laboratory, Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu 632014.
Email: krishnarao.jayaram2022@vitstudent.ac.in, pratheepkumar.a@vit.ac.in

Abstract: We describe a radical–radical cross-coupling strategy for guanylation of benzoyl-thiourea derivatives with diverse secondary amines to afford bioactive benzoyl-guanidine hybrids under blue LED irradiation in a greener reaction medium. Moreover, this effective, high-atom-economy (90%) protocol involves molecular cleavage (*via* Mumm rearrangement), formation of revised fragments, and reassembly of selective radical fragments. In addition, the work demonstrates the post-modification of benzoyl guanidine to afford bioactive isoquinolinone scaffolds via ruthenium-catalyzed oxidative annulation with diphenylacetylene.[1]

Figure/Scheme:

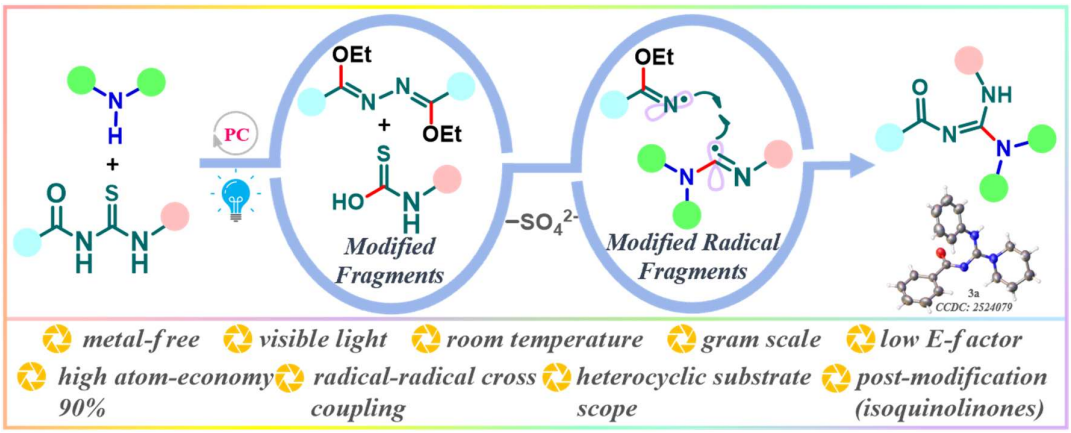

Figure 1: Graphical Abstract: An efficient and sustainable approach to access benzoyl-guanidine hybrids *via* radical–radical cross-coupling.

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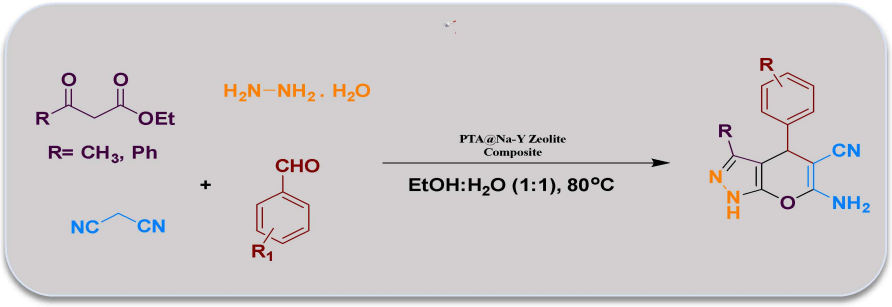
FT-8

Facile Synthesis of Pyrano[2,3-c]pyrazole Derivatives Using a Recyclable PTA@Na-Y Zeolite Catalyst: Biological Activity and DFT Studies

Priyanka Hegde, *Sib Sankar Mal**
Materials science and catalysis laboratory, Department of Chemistry, National Institute of Technology, Karnataka- 575025
Priyankakore.247cy005@nitk.edu.in

Abstract: This report details the synthesis of Phosphotungstic acid and Na-Y zeolite composite (PTA@Na-Y Zeolite) using a straightforward impregnation method. The catalytic performance of the synthesised PTA@Na-Y Zeolite was evaluated for the production of pyrano[2,3-*c*]pyrazole carbonitrile derivatives via a multicomponent reaction. The PTA@Na-Y Zeolite composite, functioning as a heterogeneous catalyst, exhibited remarkable recyclability, maintaining its catalytic activity and product yield even after seven consecutive runs. The benefits of this study include the utilisation of an efficient catalyst, reduced reaction times, improved yields, a streamlined one-pot reaction, a heterogeneous system, excellent recyclability, and a straightforward workup process. Characterisation of the synthesised catalyst was conducted using various techniques, including FT-IR spectroscopy, powder XRD, SEM, BET, ICP-MS, chemisorption, TGA, and Raman spectroscopy. Additionally, the biological activity and DFT study of the selected derivatives were assessed.

Figure/Scheme:



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FT-9

Visible-Light-Induced C-H Alkylation of Azauracil and Quinoxalinones Using Alkylboronic Acids

*Sivakumar Sudharsan, Lusina Mantry, Malati Das, and Parthasarathy Gandeepan**
Department of Chemistry, Indian Institute of Technology Tirupati, Yerpedu − Venkatagiri Road, Yerpedu Post, Tirupati District, Andhra Pradesh 517619, India
cy24d509@iittp.ac.in, pgandeepan@iittp.ac.in

Abstract: We report a visible-light-driven, pyridine N-oxide-catalyzed direct C-H alkylation of azauracil and quinoxalinones using alkylboronic acids as alkyl radical precursors. This transformation involves photoexcited 4-nitropyridine N-oxide biradical species without the use of exogenous photocatalysts. The protocol proceeds under transition-metal-free aerobic conditions, exhibits broad functional group compatibility, and accommodates structurally diverse azauracils, including functionally complex substrates. Gram-scale synthesis demonstrates the practicality and scalability of the method. Mechanistic investigations, including absorption studies, radical-trapping experiments, and NMR studies, support the generation of alkyl radicals from alkylboronic acids by photoexcited pyridine N-oxide. This operationally simple approach provides a sustainable platform for the late-stage functionalization of nitrogen-rich heterocycles relevant to medicinal chemistry.

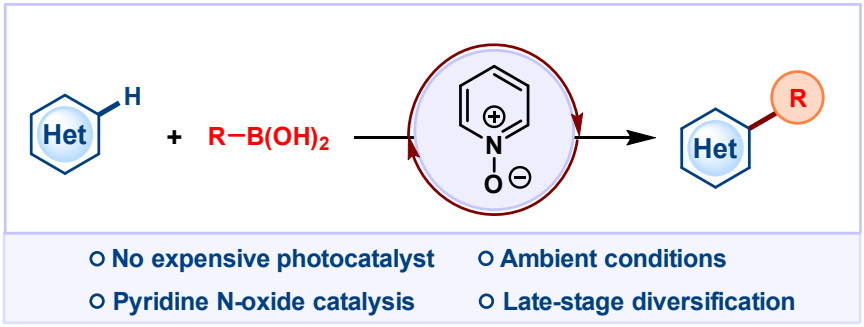

Figure 1: Visible-light-induced alkylation of heteroarenes.

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FT-10

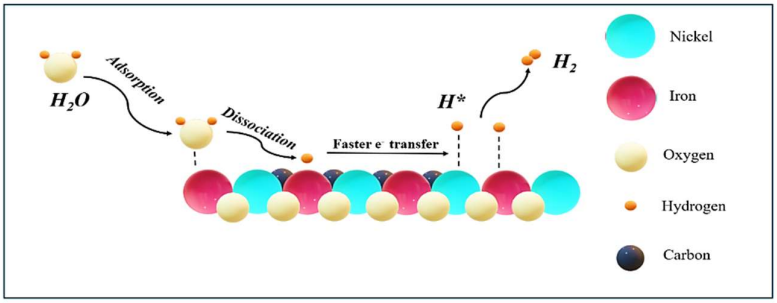
Development of In Situ Grown Transition-Metal-Based Layered Double Hydroxides Integrated with Graphene Oxide for Efficient Hydrogen Production

*Febin Benny, Nasrin Banu G, Bernaurdshaw Neppolian**

Energy & Environmental Remediation Laboratory, Department of Chemistry, Faculty of Engineering & Technology, SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamil Nadu, 603203, India.

dean.research@srmist.edu.in

Abstract: The increasing global demand for sustainable and clean energy has shifted the focus towards the production of hydrogen as a potential zero-carbon-emission fuel. In this context, hydrogen production using electrocatalytic water splitting is a highly promising method, where utilising transition metals is the most sustainable approach. NiFeLDH is a transition metal-based electrocatalyst that provides an electrochemically active surface area, which contributes to the superior catalytic activity towards water electrolysis. However, the sluggish water dissociation kinetics display relatively poor hydrogen evolution reaction (HER) activity in an alkaline medium. In order to overcome this drawback, graphene oxide is incorporated because of its high surface area and conductivity. Herein, we report a one-step hydrothermal method for the fabrication of NiFeLDH/GO@NF for HER in an alkaline medium. Systematic characterisations support the in-situ growth of the bimetallic double-layered hydroxides and the wrinkled-sheet-like structure of graphene oxide on the nickel foam surface. The as-prepared NiFeLDH/GO@NF electrode exhibits significant HER performance with an overpotential of 134 mV at 10 mA/cm^2 in 1 M KOH. This refinement in the HER activity of NiFeLDH/GO@NF can be attributed to the synergistic effects between Ni and Fe atoms as well as the high conductivity of graphene oxide. This study presents a cost-effective technique for fabricating a highly efficient NiFeLDH/GO@NF electrode and demonstrates its contribution to a green approach for hydrogen production.



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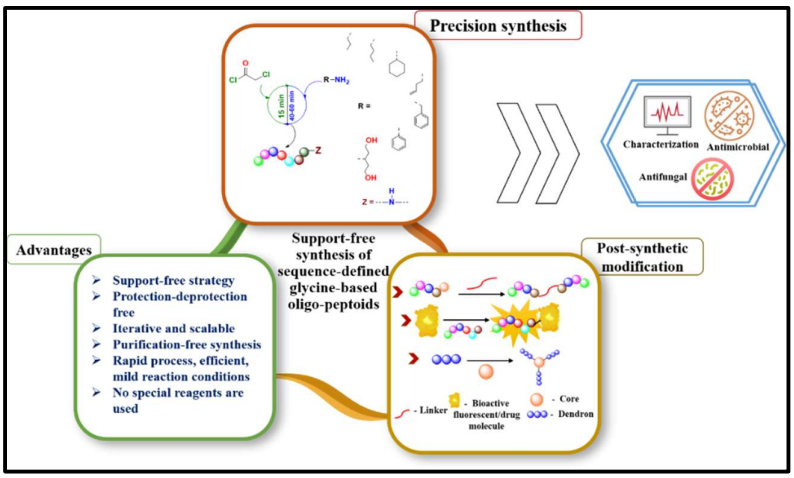
FT-11

A Modular Synthesis of Sequence-Defined Support-Free Oligopeptoids and Dendrimers for Biomedical Applications

Kavya Chellamuthu[1], *Shilpa Ravi*[2] and *Nanjan Pandurangan*[1]*
Department of Chemistry, School of Physical Sciences, Amrita Vishwa Vidyapeetham, Coimbatore -641112, Tamil Nadu, India
n_pandurangan@cb.amrita.edu

Abstract: Sequence-Defined Oligomers (SDO) emerged as a novel class of macromolecules with precisely controlled monomer sequences. However, their scalability remains challenging. Polypeptoids of N-substituted glycine backbone is a peptidomimetic oligomer possessing significant bioactivity and with improved proteolytic stability, diverging from α-carbon linkage in polypeptides. Herein, we report a novel approach for SDO synthesis, enabling several advantages, such as an iterative, support-free, protection-deprotection free, highly-efficient and scalable synthesis of N-substituted glycine-based oligopeptoids and dendrimers. A tunable comonomer and reactive amines enable rapid synthesis of 5-mer oligopeptoid *via* an amide scaffold within 9 h. As a proof of concept, we incorporated a series of alkyl and aryl groups into sequence-defined oligomers at specific sequences. Taking this into account, a synthetic approach was also developed to synthesize highly ordered, branched dendrimers. All synthesized oligopeptoids and dendrimers were extensively characterized and evaluated, showing promising antibacterial and antifungal activities. Furthermore, SAR studies reinforced by *in silico* molecular docking with influence of sequence-structural biological activity. While the peptoid oligomers showed significant bioactivity, the hydrophobic dendrimers exhibited poor aqueous dispersibility with no biological efficacy. To address these limitations, the hydrophobic dendrimers were incorporated into electrospun technique with a polymer blend generating the nanofibers which improved its bioavailability displaying antibiofilm activity and wound healing properties.



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FT-12

Active-site evolution in $CuMgAlO_x$ catalyst for hydrogen production by methanol steam reforming

Mohammed Abbas Akhtar Hasnain[a], *Porpatham Ekambaram*[b, *], *and Cheralathan Kanakkampalayam Krishnan*[a, *]

[a]*Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology (VIT), Vellore - 632 014, India*

[b]*School of Mechanical Engineering, Vellore Institute of Technology (VIT), Vellore - 632 014, India*

[*]*Corresponding author email ID: cheralathan.k@vit.ac.in (Cheralathan K K); porpatham.e@vit.ac.in (Porpatham E)*

Abstract: Methanol steam reforming (MSR) is an appealing route for producing hydrogen or hydrogen-rich reformate for energy, transportation, and industrial applications. However, the development of highly active and stable catalysts remains a key challenge. In this study, $CuMgAlO_x$ catalysts derived from Cu-Mg-Al layered double hydroxides (LDHs) with Cu loadings of 10-40 wt% were prepared to examine the combined influence of Cu content and reduction temperature on catalyst activation. Catalysts reduced at 300 °C, where only superficial CuO species were reduced, showed low initial activity that gradually increased with time on stream, indicating evolution of active sites during reaction. Post-reaction characterisation revealed structural reordering, exfoliation of the LDH layers, increased surface area, and the formation of additional Cu^0/Cu^+ species and oxygen vacancies. In contrast, catalysts reduced at 465 °C, where both superficial and bulk CuO species were reduced, exhibited immediate activity and a higher hydrogen production rate, indicating complete activation before reaction and structural stability. Moreover, increasing the reduction temperature altered the product distribution, resulting in higher CO and CO_2 selectivities than those observed for catalysts reduced at 300 °C. Among the catalysts, 30C-MAR-465 (30% Cu containing catalyst reduced at 465 °C) showed the best performance, achieving 72% methanol conversion and a hydrogen production rate of 180 $mmol/g_{cat}/h$, with stable operation for 40 h at a WHSV of 5.13 h^{-1}. Overall, the results demonstrate that the combined effects of Cu content and catalyst activation regulate the Cu^0/Cu^+ species, oxygen vacancies, and metal-support interactions, which ultimately govern the MSR activity of $CuMgAlO_x$ catalysts.

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FT-13

CVD-Grown Iron-Doped Carbon Nanoforest Beads: An Efficient adsorbent for Methylene Blue, Cadmium, and Lead Removal

*Anmol Pandey and Dr. Bhaskar Bhaduri**
Department of Chemical Engineering, Indian Institute of Technology Kharagpur
Kharagpur, 721302, India
*Corresponding author: Dr. Bhaskar Bhaduri, E-mail: bhaskar@che.iitkgp.ac.in

Abstract: Water contamination by dyes and heavy metals poses serious risks to human health and aquatic ecosystems, necessitating efficient and sustainable remediation strategies. In this study, Fe-catalyzed carbon nanoforest composite beads (Fe–CNF/Beads) were successfully synthesized via a suspension polymerization-assisted approach and evaluated for the simultaneous removal of methylene blue (MB), Pb^{2+}, and Cd^{2+} from aqueous media, river water (RW), and multicomponent systems (MB+Pb^{2+}+Cd^{2+}). The synthesized adsorbent was comprehensively characterized to examine its morphology, structural features, surface chemistry, and thermal stability. Batch adsorption experiments were conducted to investigate the effects of pH, contact time, and initial contaminant concentration. Kinetic studies revealed that the adsorption process followed the pseudo-second-order model, indicating the dominant role of surface interactions. Equilibrium data were fitted using Langmuir, Freundlich, and Redlich–Peterson (R–P) isotherms, with the R–P model providing the best fit, suggesting hybrid adsorption behavior. The maximum adsorption capacities obtained from the Langmuir model were 243.04 ± 24.79 mg/g for MB, 163.33 ± 7.98 mg/g for Cd^{2+}, and 175.51 ± 19.93 mg/g for Pb^{2+}. Fe–CNF/Beads also exhibited excellent performance in RW and multicomponent systems, together with good regeneration capability over five cycles, demonstrating their potential for practical wastewater treatment applications.

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FT-14

Room Temperature, Metal-Free, CDI-Promoted, Ex-situ Protocol for S-Methyl Thioesters Synthesis

*Manisha A. Patel[1], Vandana Sharma[1], Rupali Chavan[2], Juhi Pal[2], Santosh J. Gharpure[2], and Anant R. Kapdi[1]**

[1]Department of Chemistry, Institute of Chemical Technology, Nathalal Parekh Road, Matunga, Mumbai – 400019, India

[2]Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai – 400076, India

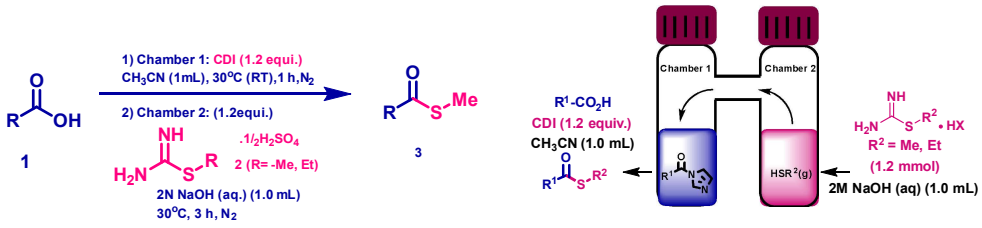
Corresponding author: ar.kapdi@ictmumbai.edu.in

Abstract: S-Methyl thioesters are essential intermediates in organic synthesis and chemical biology for their presence in key biosynthetic transformations and existence in a wide range of pharmacologically active molecules. However, there are numerous methodologies for the synthesis of thioesters, having drawbacks such as the need for metal catalysts, high temperatures, or harsh reaction conditions.

We report a mild, metal-free, room-temperature protocol for the synthesis of S-methyl and S-ethyl thioesters using carbonyldiimidazole (CDI) as a promoter in an ex-situ approach. This method provides an efficient route to a diverse library of thioesters, including aryl, heteroaryl, alkyl, and amino acid derivatives, with good to excellent yields and functional group tolerance.

Also, the methodology was successfully applied to the late-stage functionalization of commercially available pharmaceutical drugs containing carboxylic acid functionalities, enabling direct access to S-methyl thioester form. Further, we have also shown the gram-scale synthesis of one of the thioesters with the developed methodology. This approach offers a green, scalable, and operationally simple alternative to existing synthetic routes, broadening horizons for the synthesis of new bioactive compounds and prodrugs

Figure/Scheme:



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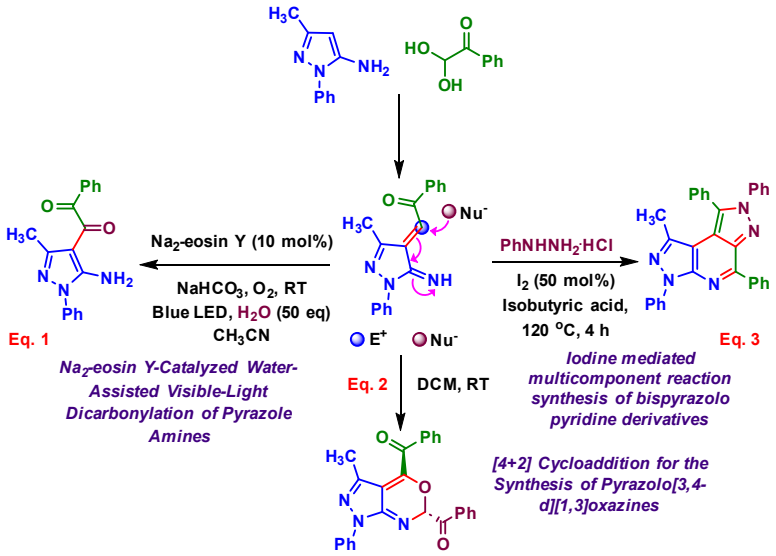
FT-15

Amphiphilic Reactivity of azole-based imino-ylidene intermediate in the Divergent Synthesis of Pyrazole Scaffolds

Karuppaiah Perumal,[a] Subburethinam Ramesh[a]*
Department of Chemistry, SASTRA Deemed University, Thanjavur-613401
Email ID: k.perumal1997@gmail.com, ramesh_s@scbt.sastra.edu

Abstract: In this work, we demonstrate the amphiphilic reactivity of an azole-based imino-ylidene intermediate, which undergoes distinct reaction pathways depending on the reaction conditions and reaction partners. Under visible-light irradiation, pyrazole amines and phenylglyoxal monohydrate undergo water-assisted oxidative dicarbonylation in the presence of water, Na_2-eosin Y, $NaHCO_3$, and molecular oxygen to afford dicarbonyl pyrazole amines (Scheme 1, Eq. 1). In the absence of light, reaction of pyrazole amine with two equivalents of phenylglyoxal provides pyrazolo[3,4-d][1,3]oxazine derivatives through a [4+2] cycloaddition pathway (Scheme 1, Eq. 2)[1]. Furthermore, in the presence of phenylhydrazine hydrochloride and iodine, the same azole-based imino-ylidene intermediate system undergoes a metal-free multicomponent transformation to furnish bis-pyrazolopyridine derivatives (Scheme 1, Eq. 3)[2].



Scheme 1: Amphiphilic Reactivity of azole-based imino-ylidene intermediate.

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FT-16

Enhanced Hydrogen Evolution Reaction Performance of α-MoO_3 Heterogeneous Catalysts for Hydrogen Evolution Reaction

K S Sandhya[1], A. Shankar Ganesh[1,*], B. A. Anandh[1], P. Nandakumar[1], K. N. Amba Sankar[2]

[1]*Department of Electronics, PSG College of Arts & Science, Avinasi Road, Civil Areodrome post, Coimbatore, Tamil Nadu, India*

[2]*Facilitation Centre for Industrial Plasma Technologies (FCIPT), Institute for Plasma Research (IPR), Bhat, Gandhinagar, Gujarat 382428, India*

Email-shankar.psgcas@gmail.com

Abstract: The increasing dependence on fossil fuels and associated environmental pollution have intensified the demand for sustainable energy technologies. Hydrogen is a promising clean energy carrier and water electrolysis offers an environmentally friendly route for its production. In this study, MoO_x and α-MoO_3 heterogeneous catalysts were synthesized chemical method and comparatively investigated for the hydrogen evolution reaction (HER). The structural and morphological properties of the synthesized catalysts were systematically characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and High-Resolution Transmission Electron Microscopy (HR-TEM). Among the investigated catalysts, α-MoO_3 exhibited superior electrocatalytic performance, requiring a low overpotential of 70 mV at 10 mA cm^{-2} current density with a tafel slope of 115 mV dec^{-1}. The α-MoO_3 catalyst exhibited an electrochemically active surface area (ECSA) of 400 cm^2. Furthermore, α-MoO_3 demonstrated excellent electrochemical stability, maintaining its catalytic performance for up to 50 h in 1.0 M KOH electrolyte. The enhanced HER activity, favourable structural and morphological characteristics and long-term stability of α-MoO_3 highlight its potential as an efficient transition-metal oxide electrocatalyst for HER performance.

Keywords: α-MoO_3, XRD, HRTEM, electrocatalysts, ECSA.

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FT-17

Hierarchical porosity induced monolithic viologen-based Covalent Organic Frameworks for ultrafast removal of pollutants from water/ Pollution remediation

Arjun Warrier [a] Pampa Jhariat [a] Mebin Varghese [a] and Tamas Panda[b]*

[a] *Department of Chemistry, Vellore Institute of Technology, Vellore, Tamil Nadu-632014*

[b] *Centre for Clean Environment, Vellore Institute of Technology, Vellore, Tamil Nadu-632014*

Abstract: Hierarchically porous adsorbents that combine rapid mass transport, structural robustness and scalable processability are highly desirable for practical water purification. Two-dimensional covalent organic frameworks (COFs) possess intrinsic microporosity and tunable functionality. However, translating these crystalline materials into continuous macroscopic architectures with accessible multiscale porosity remains a significant challenge. Here, we report a simple self-shaping gas-foaming strategy for the rapid synthesis of monolithic viologen-based COFs with hierarchical porosity. The resulting monolith (denoted mL3Tp, m = monolithic) is synthesized by an industrially compatible ball-milling method completed within 10 min. In situ gas-phase foaming induces heterogeneous pore nucleation, disrupts ordered two-dimensional crystallite growth, and generates an interconnected three-dimensional porous network spanning micro-, meso- and macroporous regimes, as confirmed by micro-computed tomography. To our knowledge, this is the first self-shaped monolithic viologen-based COF fabricated through a gas-foaming approach. The hierarchically porous mL3Tp monolith exhibits ultrafast and highly efficient removal of inorganic oxoanions (MnO_4^-, ReO_4^-, CrO_4^{2-} and $HAsO_4^{2-}$) and anionic organic dyes, achieving >99% removal within ~10–60 s depending on the contaminants. The monolith can be produced at bulk scale and reused over at least five cycles without significant loss of performance. Notably, mL3Tp effectively removes As(V) and Cr(VI) from naturally contaminated groundwater samples collected from different regions of India, reducing concentrations below World Health Organization (WHO) limits. Density functional theory calculations reveal strong non-covalent host-guest interactions underlying the rapid adsorption behaviour, highlighting the promise of self-shaped monolithic COFs for scalable water remediation.

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FT-18

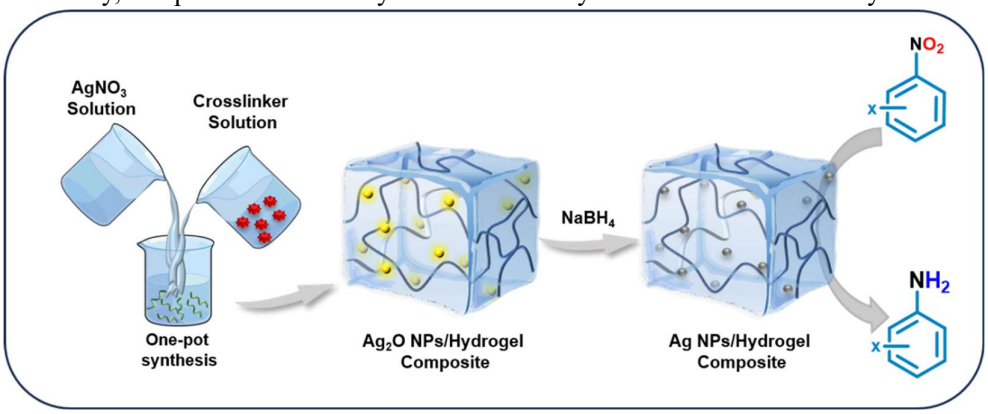
Greener & Faster: Recyclable Alginate Hydrogel-Supported Ag Nanoparticles for Rapid Nitroarene Reduction

Damini Jagankar *and Chandan Maity**

(Organic)Material Science and Engineering Laboratory, Department of Chemistry, School of Advanced Sciences (SAS), Centre for Nanobiotechnology (CNBT), Vellore Institute of Technology (VIT), Vellore Campus, Tamil Nadu-632014, India, **Email:** chandan.maity@vit.ac.in (CM)

Nitroarenes are persistent environmental contaminants due to their chemical stability and inherent toxicity. Their conversion into corresponding aryl amines is environmentally and industrially important, as these products are less hazardous and serve as valuable intermediates in pharmaceuticals, agrochemicals, and advanced materials.[1] However, conventional nitroarene reduction methods often employ hazardous reducing agents, generate significant chemical waste, and require harsh reaction conditions. Moreover, catalyst recovery and reuse remain challenging, limiting the sustainability of these processes.[2,3]

In this presentation, we will describe how a recyclable alginate hydrogel-supported silver nanoparticle (Ag NPs) composite enables rapid reduction of structurally diverse nitroarenes under mild aqueous conditions.[4] Ag_2O nanoparticles were generated *in-situ* within the alginate hydrogel network and subsequently converted into catalytically active Ag NPs using aqueous $NaBH_4$. The hydrogel matrix effectively stabilizes the nanoparticles, minimizes aggregation, facilitates catalyst recovery and reuse, and promotes efficient mass transfer during catalysis. The resulting composite efficiently converts a broad range of nitroarenes to their corresponding amines in water at room temperature within 15–30 min using a low amount of $NaBH_4$. This simple and recyclable catalytic platform offers a greener and faster approach to nitroarene reduction, combining mild aqueous processing, rapid conversion, facile catalyst recovery, and potential scalability for sustainable synthesis of value-added aryl amines.



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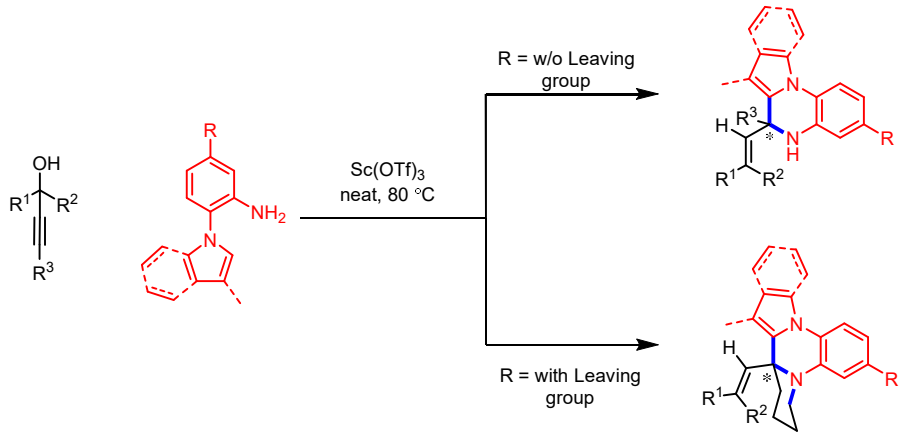
FT-19

Lewis-Acid Catalyzed Regioselective Annulation Synthesis of Trisubstituted Alkenes Bearing a Quaternary Carbon Cyclic Fused Quinoxaline

Avinash Kumar, *Srinivasarao Yaragorla**
School of Chemistry, University of Hyderabad, Hyderabad, 500046, India
**E-mail: srinivas.yaragorla@uohyd.ac.in*

Abstract: A Lewis-catalyzed cyclization strategy has been developed to synthesize biologically significant nitrogen-containing heterocycles, including pyrrolo[1,2-a]quinoxalines, indolo[1,2-a]quinoxalines[1,2], and tetrahydro-10H-pyrido[1,2-a]pyrrolo[2,1-c]quinoxalines having trisubstituted alkenes bearing a quaternary carbon. These compounds are constructed from readily accessible tertiary propargylic alcohols and 2-pyrrolyl or 2-indolyl arylamines. The method involves allene formation followed by intramolecular [5+1] annulation or intramolecular [5+1] annulation followed by intramolecular nucleophilic substitution yielding a diverse range of quinoxaline derivatives with trisubstituted alkenes, excellent regioselectivity, and moderate diastereoselectivity. Additionally, gram-scale synthesis, synthetic transformations, and mechanistic insights based on intermediate isolation have been demonstrated.



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FT-20

Development of biopolymer-based Ocular Films for Prolonged Neuro-related chronic Dry eye disease Delivery

Sowmiya.R[1], *B. Siva Kumar*[1]*, *Sarda Sharma*[1], *S. Giridhar Reddy*[1], *Sangly P.Srinivas*[2]

[1]*Amrita School of Engineering, Amrita Vishwa Vidyapeetham, Bangalore, 560035, India*

[2]*School of Optometry, Indiana University, Bloomington, Indiana, 47405, USA*

[*] *b_sivakumar@blr.amrita.edu*

Abstract: Traditional eye drops face major challenges due to rapid washout, requiring frequent application, which often leads to lower bioavailability, non-adherence and larger dose requirement in patients. To overcome these limitations, a biocompatible ocular film insert was developed to enhance drug (gabapentin) delivery in neuropathic-based dry eye disease (DED). This formulation was designed specifically around the anatomical dimensions and physiological conditions of the human eye, with a focus on the anterior eye. The inserts were prepared via a solvent-casting method utilising a biopolymer matrix. Mechanical testing demonstrated that the films easily withstand the stresses required for safe and effective ocular administration. The physicochemical characterisations confirmed that this optimised formulation exhibited excellent uniformity in mass, thickness, and drug content, in strict accordance with pharmaceutical standards. Ultimately, this study introduces an innovative, anatomy-based experimental framework for testing new advanced ocular drug delivery systems. [1], [2], [3], [4]

Keywords: *Ocular drug delivery, gabapentin, Biopolymer, DED*

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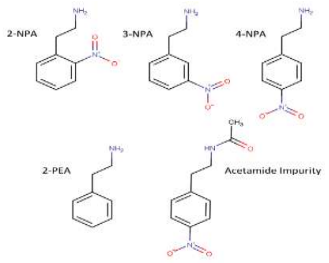
FT-21

Sustainable Analytical Development Approach: RP-HPLC Method for Simultaneous Quantification of Substituted Isomers of 4-Nitrophenylethylamine and Related Impurities

Sanjay Kumar Sharma[1,2], *Prof. Sayeeda Sultana*[2],
[1] *Research Scholar, Department of Chemistry, St. Peter's Institute of Higher Education and Research, Avadi, Chennai, 60054, Tamilnadu, India.*
[2] *Department of Chemistry, St. Peter's Institute of Higher Education and Research, Avadi, Chennai, 60054, Tamilnadu, India.*

Abstract: Para nitro phenyl ethylamine (4-NPA) is a key starting material, which is used in manufacturing for many of the drug substances, and is synthesized from 2-Phenyl ethylamine (2-PEA). In 4-NPA synthesis, 2-nitrophenylethylamine (2-NPA) and 3-nitrophenylethyl amine (3-NPA) are generated as by-products which are positional isomers. Along with this, one of the process impurities forming is 4-Nitrophenylethylacetamide (Acetamide Impurity). The HPLC methodology showed a good linearity, good system precision and good method precision. This method can be used to assess the quality of 4-NPA sample for the presence of 2-NPA, 3-NPA, 2-PEA, acetamide impurity. AGREE tool is a green analytical software that can be used with any analytical technique to assess the environmental friendliness of the developed analytical procedures. The software supports green analytical chemistry regarding sample handling, derivatization, mechanization, simplification, solvent safety study, quality of sample used for analysing, various components quantified in one analysis and energy consumption per run. It is established based on these 12 important elements of relating analysis with methodology [13].

Key words: PFP Column, Gradient mode, High-pressure liquid chromatography, Positional Isomers, Para nitrophenylethylamine, Sustainable approach. **References:**



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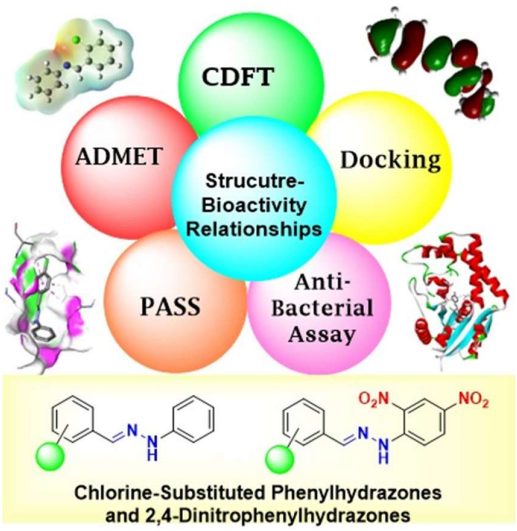
FT-22

Structure–Bioactivity Relationships in Chloro-Substituted Phenylhydrazones: CDFT, In Silico, and Antibacterial Studies

P. Jenifer Jasmine Mary and A. Irudaya Jothi
Department of Chemistry, St. Joseph's College, Tiruchirappalli 620002, Tamil Nadu, India.

Abstract: Molecular framework and substituent topology are key determinants of the physicochemical, pharmacokinetic, and biological properties of hydrazone derivatives. In this study, the individual effects of molecular framework and chloro regioisomerism were investigated through a comparative analysis of regioisomeric phenylhydrazones (PHs, **1**–**4**) and their corresponding 2,4-dinitrophenylhydrazones (DNPHs, **5**–**8**). Structure–property–bioactivity relationships were explored using conceptual density functional theory (CDFT), PASS-based bioactivity prediction, molecular docking, ADMET evaluation, and in vitro antibacterial assays. CDFT calculations at the B3LYP/6-311++G(d,p) level revealed enhanced electron affinity and electrophilicity for the DNPH derivatives relative to the corresponding PHs. PASS prediction and molecular docking identified adenosylmethionine decarboxylase (ADMATase) as a promising biological target, with the DNPH framework exhibiting stronger binding interactions, while chloro substitution modulated ligand–protein interactions in a position-dependent manner. ADMET analysis indicated superior drug-likeness and membrane permeability for the PH series, whereas the DNPH analogues displayed increased polarity. Experimental antibacterial studies demonstrated consistently higher activity for the PH derivatives, particularly against Gram-positive bacteria, highlighting the dominant influence of molecular framework over chloro regioisomerism on biological performance. These findings provide molecular-level insights into the interplay between scaffold architecture, electronic structure, pharmacokinetics, and antibacterial activity in hydrazone systems. This integrated study provides valuable insights into how scaffold effects, chlorine substitution, and regioisomerism collectively govern the structure–property–activity relationships of phenylhydrazone systems, while supporting United Nations Sustainable Development Goal 3 (Good Health and Well-Being) through the comprehensive evaluation of hydrazone derivatives using molecular modelling, toxicity prediction, and antibacterial assessment.



Keywords: Diaryl Schiff bases; Methoxy substitution; regioisomerism; Solvatochromism; Conceptual DFT: Nonlinear optical (NLO) properties.

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Poster Presentation - PP

PP-1

Sustainable Bio-Derived Dynamic Hydrogels from Polyvinyl Alcohol and Carboxymethyl Cellulose for Air Pollutant Capture and Environmental Remediation

Bhoomish Somasundaram and Dr. Vijayalakshmi Shankar*

School of Chemical Engineering, Vellore Institute of Technology, Vellore – 14, India
School of Healthcare Science and Engineering, Vellore Institute of Technology, Vellore – 14, India

Abstract: The increasing concentration of greenhouse gases and acidic air pollutants represents a critical challenge for global climate stability and environmental sustainability. The development of sustainable, organic materials capable of efficiently capturing carbon dioxide (CO_2) and reducing airborne emissions is therefore essential for energy-efficient environmental remediation. In this study, we report the fabrication of a bio-derived dynamic hydrogel based on polyvinyl alcohol (PVA) and carboxymethyl cellulose (CMC) for the targeted capture of CO_2 and other acidic air pollutants. The incorporation of dynamic hydrogen-bonding and amine linkages imparts regenerability, and pH-responsive characteristics to the polymer network, enabling repeated pollutant capture and release cycles with a low energetic penalty. By facilitating reversible carbon capture, the developed hydrogel offers a pathway to mitigate greenhouse gas accumulation while supporting circular carbon economy initiatives. This sustainable PVA-CMC hydrogel platform represents a cost-effective, organic approach for atmospheric carbon reduction and broad environmental remediation. Ultimately, this work demonstrates a simple, scalable, and eco-friendly framework, providing a promising materials-driven strategy for addressing the interconnected challenges of environmental remediation and energy sustainability.

Keywords: Polyvinyl Alcohol, Carboxymethyl Cellulose, Air pollutant capture, Hydrogen-bonding, Amine functionalization, Carbon dioxide adsorption, Environmental remediation, Carbon Reduction, Dynamic hydrogels.

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PP-2

Comparative Performance and Sustainability Assessment of Chemical and Algal Biocatholytes in Microbial Desalination Cells under Continuous Operation with Integrated Biomass Valorization for a Zero-Waste Management

Dhandapani Murugan*[a], *Kalaichelvi Ponnusamy*[a], *Samsudeen Naina Mohamed*[a]
[a]Department of Chemical Engineering, National Institute of Technology Tiruchirappalli, India
Corresponding Author: samsudeen@nitt.edu

Abstract: Microbial desalination cells (MDC) are emerging bioelectrochemical technologies developed for simultaneous electricity production and wastewater treatment, along with desalination. In this present study, the performance and sustainability of the various catholytes, including $KMnO_4$, potassium persulfate, phosphate-buffered saline, and an algal biocatalyst, were evaluated under neutral and unneutralized conditions during continuous MDC operation. This study also evaluates the potential of biocatholytes as sustainable alternative to conventional chemical and buffer catholytes. Among the tested catholytes, $KMnO_4$ exhibited superior performance and achieved the maximum power density of 359.1± 8.6 mW/m², while PPS, BC, and PBS achieved maximum power densities of 107.6 ± 5.2 mW/m², 73.5 ± 4.3 mW/m², and 58.2± 3.7 mW/m², respectively. Despite Its lower power output, PPS, exhibited higher desalination and organic removal performance, achieving a maximum of 40.81 ± 21% and 81.16 ± 11%, respectively. The overall performance order for desalination and COD removal was PPS > $KMnO_4$ > PBS > BC. In this study, chemical catholytes showed enhanced MDC performance; however, their performance declined during long-term operation due to their potential loss. While the biocatholytes showed superior performance and simultaneously generated valuable biomass throughout the long term operation. Subsequently, the recovered biomass was utilized for various bioproduct production and yield a total of 2.63 mg/g of phycobiliproteins, 91.08 µg/mL of total pigments, 0.33g/g biofuel, and 33.75 % biochar. These findings demonstrate the feasibility of integrating algae in MDC operations and Support the zero-waste management and sustainable recovery approach.

Keywords: Microbial Desalination Cell, Chemical Catholytes, Biocatholytes, Biomass Valorization.

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PP-3

Eco friendly removal of Rhodium B from waste water using green synthesised MgO nanoparticles from Azadirachta indica

Eashwatha R[a], Narmadha R[b], Dhinesh D[c] and

Rajabhuvaneswari Ariyamuthu[d*]

[a,b,c]*Department of Biotechnology, Karpaga Vinayaga College of Engineering and Technology, Karpaga Vinayaga Educational Lore for Learning (Deemed to be University) GST Road, Chinna Kolambakkam, Maduranthagam(Tk), Kancheepuram Dist., TN, India- 603 308*

[d]*Department of Chemistry, Karpaga Vinayaga College of Engineering and Technology, Karpaga Vinayaga Educational Lore for Learning (Deemed to be University) GST Road, Chinna Kolambakkam, Maduranthagam(Tk), Kancheepuram Dist., TN, India- 603 308*

ABSTRACT: Industrial effluents containing refractory synthetic dyes are considered one of the most significant threats to water bodies such as global aquatic systems and municipal water security. Besides, advanced remediation strategies, the emergence of of magnesium oxide (MgO) nanoparticles (NPs) through neem leaf extract (Azadirachata indica) and precursor of magnesium sulfate heptahydrate (MgSO4.7H2O). Synthesis conditions were optimized systematically from precursor to extract volumetric ratio (1:1, 2:3 and 3:4) and calcination temperature range are 200° C and 400° C. The highly stable yield of nanostructured MgO with reduced particle dimension formed at 3:4 volumetric ratio with calcination at 400° C. Fourier-Transform Infrared Spectroscopy (FTIR) confirmed the formation of metal-oxygen lattice formation (MgO bending at 598 cm-1) associated with residual hydroxyl (3468 cm-1) and carbonyl groups (1372 cm-1 and 1678 cm-1) through phytochemical shows behaviour of stabilizing behaving agentsensuring functional surface interactions with Rhodamine B (RhB). The systematic evaluations study study of batch adsorption about the impacts of initial dye concentration (5 - 20 ppm), contact time (1 - 3 hrs) and pH (5, unadjusted and 9). Maximum dye removal under acidic conditions (pH 5), efficiency reached 64.6% for the concentration 5 ppm RhB after 3 hrs of contact time, for 20 mL 10 mg of adsorbent dosage were used. Performance degradation can be observed in alkaline medium (pH 9) and under equivalent loading maximum yield obtained is only 24.3% due to competitive inhibition of hydroxyl ion (OH-) and electrostatic repulsion. Overall, biogenically stabilized MgO NPs show strong potential as sustainable adsorbents for specific decontamination of textile water discharge.

Keywords : MgO nanoparticles, Green synthesis, Neam leaf extract (*Azadirachta Indica*), Rhodamine B, dye degradation

PP-4

Engineered Chitosan-Polyurethane Composite Foams as Versatile Absorbents for Toxic Heavy Metals

Lakshmi K, Boominathan T, Indresh Singh, Dr. E. Veera Venkata Ramesh and Dr. Akella Sivaramakrishna**

Department of Chemistry, School of Advanced Sciences, VIT, Vellore 632014, TN

asrkrishna@vit.ac.in

Abstract: The escalating concern for environmental protection and water security has driven the search for sustainable adsorbents capable of eliminating toxic contaminants efficiently from aqueous systems. [1,2] In this study, we demonstrate the successful development of functionalized chitosan-dependent polyurethane foams (PUCS-GP, PUCS-CA-GP, PUCS-TA-GP, and PUCS-GA-GP) as versatile platforms for the removal of both anionic and cationic heavy-metal species, including dichromate ($Cr_2O_7^{2-}$), Cr(III), Cd(II), and Pb(II). Systematic batch adsorption experiments were conducted to elucidate the effects of solution pH, adsorbent dosage, initial ion concentration, contact time, and temperature on sorption performance. Kinetic analyses revealed that the adsorption process conforms to a pseudo-second-order model, with maximum uptake capacities of 23.67 mg g^{-1} for dichromate on PUCS-GP at pH - 2, and 22.29, 22.02, and 23.07 mg g^{-1} for Cr(III), Cd(II), and Pb(II), respectively, on PUCS-CA-GP at pH 6 under ambient conditions. Equilibrium data were well described by Langmuir, Freundlich, and Temkin isotherm models, while thermodynamic parameters provided mechanistic insight into the adsorption pathways. Importantly, regeneration studies confirmed that dichromate- and metal-loaded foams retained >90% removal efficiency over eight adsorption-desorption cycles, underscoring their recyclability and operational stability. Notably, these PUCS-based foams are promising candidates for sustainable heavy-metal remediation, high sorption capacity, and exceptional reusability.

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PP-5

Evaluation of cellulolytic enzyme production by *Aspergillus niger* under solid state fermentation using agricultural waste

*L A Swagatika Priyadarshini, Rashmi Kataria**
School of Biosciences and Technology
Vellore institute of technology, Vellore, Tamil Nadu, India, 632014
swagatikapriya@vit.ac.in
rashmi.kataria@vit.ac.in

Abstract: The sustainable utilization of lignocellulosic biomass for the industrial enzyme production has gained a considerable attention due to its economic and environmental benefits. Coconut biomass is an abundant agro-industrial residue that represents a suitable substrate for the production of hydrolytic enzyme through solid state fermentation (SSF). The recalcitrant lignin matrix of untreated biomass restricts microbial colonization and enzyme secretion. In present study, untreated and alkali pretreated coconut biomass were used as substrate for the enzyme production by *Aspergillus niger* under SSF. Fermentation was carried out under optimized conditions and crude enzyme extracts were recovered for biochemical characterization. Ther maximum CMCase activity increased from 0.307 IU/mL (day 9) in untreated biomass to 1.027 IU/mL (day 9) in alkali pretreated biomass. The findings of this study highlight the potential of alkali pretreated coconut biomass as an efficient low-cost substrate for the production of industrially important enzymes. This work contributes to valorisation of coconut residues and supports the development of sustainable bioprocess for biomass conversion.

Keywords: *Aspergillus niger*, solid state fermentation, coconut biomass, alkali pretreatment, cellulase, amylase, lignocellulosic biomass

PP-6

Analytical Technique For The Development And Validation Of A Sensitive Reverse Phase Hplc Method For Determination Of Hydrazine In An Active Pharmaceutical Ingredients

LOKESH[1,2]✉, SAYEEDA SULTANA[2*]

[1]Research Scholar, Department of Chemistry, St. Peter's Institute of Higher Education and Research, Avadi, Chennai-60054, Tamilnadu, India

[2]Department of Chemistry, St. Peter's Institute of Higher Education and Research, Avadi, Chennai-60054, Tamilnadu, India.

Corresponding author: lokeshravi1711997@gmail.com

Abstract: Hydrazine is a vital intermediate in organic synthesis, utilized in various applications including the production of Pimobendan. This study focuses on the impurity analysis of Hydrazine on green approach, with particular emphasis on the detection and quantification of hydrazine. A high-performance liquid chromatography (HPLC) method was developed using a Inertsil 3V(4.6*250mm*5µm) column and optimized for resolution and sensitivity. The method demonstrated effective separation, with detection limits for hydrazine in Pimobendan. The analytical method also been validated as per the stipulations of ICH guideline values and to furnish a method which within the permissible limit as per specified in ICH M7 guidelines regarding the analytical guideline for estimation of genotoxic impurities. The validation study data imparts feasible and reliable use of this method to analyze for the quality control to determine the hydrazine content in trace levels in the API product.

Keywords: Green approach, Hydrazine, RP HPLC, Genotoxic impurity

PP-7

Molecular Level Insights into the Stability of Unnatural Base Pairs in DNA Duplex: A Computational Approach

Malavika Jayan, Dr. *Tanay Debnath*
Dept. of Chemistry, SAS, VIT Vellore.

Abstract: The genetic information in living organisms is encoded by 4-letter nucleotide alphabet, which, when read as triplet codons, provides 64 possible codons for the coding of 20 amino acids. The development of an expanded genetic alphabet through the incorporation of Unnatural Base Pairs (UBPs) offers a promising approach to increase the information capacity of DNA and enable the encoding of additional genetic information. Significant advances in UBP development have been achieved by the research groups of S. A. Benner, Ichiro Hirao and Floyd Romesberg, leading to chemically diverse UBP systems with distinct structural and recognition properties. However, the stability and behaviour of an isolated UBP can differ substantially from its behaviour within the highly constrained environment of a DNA duplex. Therefore, understanding the molecular factors governing UBP stabilization in both isolated and DNA- incorporated state is essential for the rational design of efficient UBPs.

In the present study, we computationally investigate the structural and energetic stabilization of Romesberg's d5SICS-dNaM and dTPT3-dNaM UBP systems and explore their potential as scaffolds for the design of new UBP candidates. The effects of different substitutions on UBP stability were systematically evaluated using Density Functional Theory (DFT) and Symmetry-Adapted Perturbation Theory (SAPT) calculations. Particular emphasis was placed on the changes in interaction energies and the preferred intercalated geometries resulting from these modifications. Furthermore, QM/MM calculations were employed to examine the structural stabilization of the DNA duplex upon incorporation of UBP. This combined computational approach provides the relationship between chemical substitution, intermolecular interactions, preferred UBP geometry and stabilization within the DNA environment, thereby establishing molecular level insights useful for the rational design and optimization of UBPs.

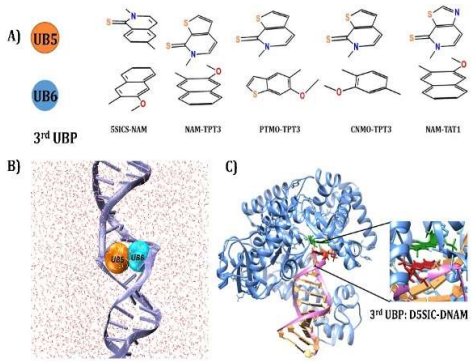

Figure: A) Schematic representation of hydrophobic UBPs; B) UBP incorporated DNA structure; C) UBP incorporated DNA bound to protein system.

PP-8

Accelaerated Cr(VI) Remediation Using Layered Zinc Acetate

Sibiya Stacey R G, Saranya S, Mariya T B, Aarthi S, *Buvaneswari G**
Department of Chemistry, Vellore Institute of Technology, Vellore, Tamil Nadu, India
Email: gbhuvaneswari@vit.ac.in

Abstract: Industrial discharge of toxic hexavalent chromium, Cr(VI), remains as one of the most pressing environmental challenges due to its high toxicity, carcinogenicity, mobility and persistence in aquatic ecosystems. Hence it is important to completely remove Cr(VI) from wastewater. Conventional remediation strategies face limitations including high operational costs, slow kinetics, or require complex materials. Here we address these gaps, by introducing a simple layered zinc acetate that efficiently removes large concentration of Cr(VI). The study of physio-chemical nature of the synthesized material were done by characterization techniques such as Powder X-Ray Diffraction (P-XRD) and Fourier Transform Infrared Spectroscopy (FT-IR). The effect of various reaction parameters including pH, amount of adsorbent, initial concentration of Cr(VI) and kinetics were investigated and the material performed exceptionally well in immobilizing high concentrations of Cr(VI) rapidly. The material showcased an exceptional performance of 98% removal for 100 mg/L of Cr(VI) under 15 min.

Figure: Flow of carcinogenic hexavalent chromium

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PP-9

Functionalized ammonia-borane mediated synergistic metal-free strategy for the Water-Gas shift reaction: A systematic DFT study

Suphal Sen[a], *Tanay Debnath*[a]*
[a]*School of Advanced Sciences, Vellore Institute of Technology, Vellore, TN, 632014, India*
[*]*To whom all correspondence should be addressed*
Email: tanay.debnath@vit.ac.in

Abstract: Syngas, a mixture of carbon monoxide (CO) and hydrogen (H_2), is an important feedstock for the sustainable production of fuels and value-added oxygenated chemicals. In this work, density functional theory (DFT) calculations were employed to investigate a series of functionalized ammonia-borane derivatives, $NH(R_1)_2BH(R_2)_2$, as metal-free hydrogen-storage reagents for the sequential conversion of CO through coupled hydrogenation and water-gas shift reaction (WGSR) pathways[1]. The complete reaction network comprises ammonia-borane-mediated hydrogenation of CO to formaldehyde (HCHO), hydrolysis of the ammonia-borane derivative, hydrolytic conversion of CO to formic acid (HCOOH), and decomposition of HCOOH to CO_2 and H_2 for catalyst regeneration[2,3]. The generated HCHO can subsequently undergo further hydrogenation to methanol (CH_3OH), thereby establishing an integrated route for syngas valorization. A systematic structure-activity relationship study was performed by varying the substituents on both the nitrogen and boron centers of the ammonia-borane framework, and the reaction energetics were analyzed at the level of individual elementary steps as well as for the complete one-pot catalytic cycle. The calculations reveal that functionalization of the ammonia-borane scaffold strongly influences the thermodynamic and kinetic characteristics of CO activation, hydrogen transfer, hydrolysis, and catalyst regeneration processes. Among the investigated systems, cyclic π-conjugated aromatic ammonia-borane derivatives bearing electron-donating substituents on boron and electron-withdrawing substituents on nitrogen exhibit the most favorable balance of activation barriers, reaction free energies, and regeneration efficiency. Overall, this study establishes a mechanistic framework for the metal-free conversion of syngas-derived CO into formaldehyde and methanol through ammonia-borane-mediated hydrogenation coupled with WGSR chemistry and provides valuable molecular design principles for developing sustainable and cost-effective catalysts for carbon monoxide utilization.

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PP-10

Optimal Bandwidth in Semiconducting Polymer Chains

Suryoday Prodhan[1]*, *Alessandro Troisi*[2]*

[1]*Department of Chemistry, Birla Institute of Technology and Science, Pilani, Hyderabad Campus, Telangana 500078, India*

[2]*Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, UK*

suryoday.prodhan@hyderabad.bits-pilani.ac.in

Abstract: Systematic development of polymeric semiconductors has seen a general trend over the last four decades, where band narrowing has emerged as a suitable recipe for improving the charge transport characteristics.[1] However, this strategy cannot be extended indefinitely since vanishing bandwidth will result in vanishing charge mobility. Experimental and theoretical investigations have also hinted towards a shift in the transport regime as the carrier band becomes narrower.[2] In a recent work, we demonstrate that narrowing the band beyond a certain threshold modifies the nature of the charge-carriers, from partially delocalized to fully localized, and this transition corresponds to the maximum achievable mobility.[3] Employing a fully controllable model, we illustrate that the current state-of-the-art polymers remain in the 'sweet spot' of the bandwidth and that further reduction in electronic coupling will not improve charge mobility significantly.[3]

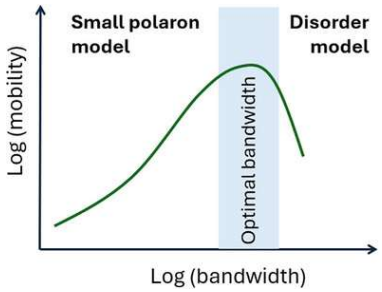

Figure 1. Combined polymer bandwidth versus hole mobility profile. The polaron is fully localized (delocalized) at smaller (larger) bandwidth and the transition between these two regimes represents the optimal bandwidth which corresponds to maximum in polymer charge mobility (blue shaded region).

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PP-11

DEVELOPMENT OF A STABILITY INDICATING HEADSPACE GAS CHROMATOGRAPHIC METHOD FOR DETERMINATION OF CARCINOGENIC BENZENE IN MULTIPLE ACTIVE PHARMACEUTICAL INGREDIENTS WITH COMPREHENSIVE RUGGEDNESS ASSESSMENT USING ANALYTICAL QUALITY BY DESIGN

Vigneshwaran[1,2]✉, Sayeeda Sultana[1*]

[1,2]Research Scholar, Department of Chemistry, St. Peter's Institute of Higher Education and Research, Avadi, Chennai, 60054, Tamilnadu, India.

[2*]Department of Chemistry, St. Peter's Institute of Higher Education and Research, Avadi, Chennai, 60054, Tamilnadu, India.

✉E-mail address: vickysaraswathy18@gmail.com

Abstract: Benzene is a substantial solvent which is carcinogenic and class-1 critical solvent that need to be be estimated precisely in the drug sample of human and veterinary API. It is vastly used in various organic and chemical synthesis reaction as reactant to obtain the product. It is widely used in the reactions of API drug formation to get the desired drug. In this research study the focus is primarily on the ruggedness of the Benzene content method developed in gas chromatography in three dipersive API drugs. A Gas Chromatography (GC) method was established using a DB-1 (60m × 5 mm, 3.5 µm) column. The established method demonstrated effective dispersion, with detection limits for benzene at low levels and high levels respectively. The validated GC method impart reliable analysis for the estimation of benzene content in the sample at trace levels, ensuring identification and quantification of low impurity levels in the final product of API and it can be imparted in any drugs. Established method furnish on exact quanitification of critical benzene content in the API Drugs with clear separation and resolution of benzene from the analyzed data.

Keywords: Benzene, GC, Carcinogen impurity

PP-12

Design, Synthesis, Molecular Docking, and In vitro Antiproliferative Evaluation of Quinoline-Pyranocoumarin Hybrids as Potent DNA Topoisomerase II Inhibitors

Amruta K. Durgi, Aravind Krishnan, and Ajesh Vijayan*
Department of Chemistry, Christ University, Bangalore, 560029, India
Email: ajesh.vijayan@christuniversity.in

Abstract: Quinoline and coumarin scaffolds are well-established pharmacophores with diverse biological activities, including promising anticancer properties.[1] In the present study, a series of novel quinoline–pyranocoumarin hybrids (4a–4j) was designed, synthesized, and evaluated as potential DNA topoisomerase IIα inhibitors.[2] The target compounds were synthesized through an optimized one-pot protocol and structurally characterized using FT-IR, ^{1}H NMR, ^{13}C NMR, and mass spectrometry. Molecular docking studies against human DNA topoisomerase IIα (PDB ID: 5GWK) identified compound 4b as the most promising derivative, exhibiting a binding affinity of −8.02 kcal/mol, surpassing the reference drug doxorubicin. The antiproliferative potential of compound 4b was subsequently investigated in MCF-7 and K562 cancer cell lines using in vitro cell viability assays. Compound 4b demonstrated enhanced cytotoxic activity, with greater potency against MCF-7 cells. Flow cytometric cell cycle analysis further revealed significant G_2/M phase arrest in MCF-7 cells following treatment with compound 4b, supporting its mechanism of action through topoisomerase II inhibition. Collectively, these findings identify quinoline– pyranocoumarin hybrid 4b as a promising lead molecule for the development of novel anticancer agents targeting DNA topoisomerase IIα.

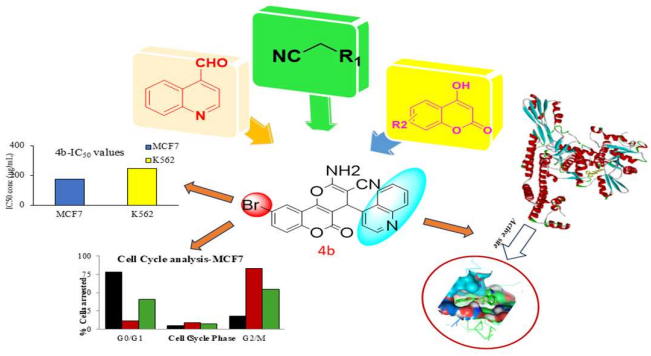

Figure: Synthetic Strategy and Biological Evaluation of Quinoline–Pyranocoumarin Hybrids

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PP-13

One-pot synthesis of α-(OCH_2CF_3)-substituted pyridines using TFE as both a solvent and a reagent

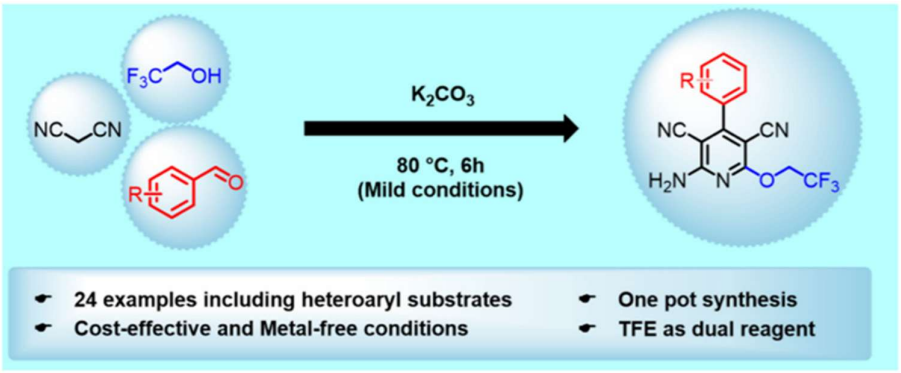
Anilkumar Kommoju, [b] Kishor Padala *[b] and Togati Naveen *[a]

[a]Department of Chemistry, Sardar Vallabhbhai National Institute of Technology Surat, Gujarat-395 007, India. E-mail: togatinaveen123@gmail.com

[b]Department of Chemistry, Central Tribal University of Andhra Pradesh, Vizianagaram, Andhra Pradesh, 535003, India. E-mail: kishor.padala@gmail.com.

Abstract: Trifluoroethoxy-substituted pyridines are among the core components of many biologically active scaffolds and have a wide range of applications in fields such as materials science, agrochemicals, and pharmaceuticals. The strategic placement of fluorine-containing substituents, like the 2,2,2-trifluoroethoxy group in the target compound, is a crucial aspect of modern drug design. This group can act as a lipophilic hydrogen-bond donor and participate in favourable interactions with biological targets. Here, we developed a novel and efficient method for synthesizing α-(OCH_2CF_3)-substituted pyridine-3,5-dicarbonitriles from readily available starting materials such as benzaldehydes, malononitrile, and trifluoroethanol (TFE), using a base. In this process, TFE serves a dual role as both the solvent and the source of the trifluoroethoxy group. Delightfully, diverse substituted benzaldehydes were efficiently transformed into the corresponding trifluoroethoxy-substituted pyridines in 54–95% yields. The reaction proceeds under mild conditions, avoids the need for pre-functionalized substrates, and exhibits broad functional group tolerance, providing a practical method for synthesizing diverse trifluoroethoxy-substituted pyridines.[1]

Figure/Scheme:



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PP-14

Visible-Light-Induced Thiocyanation of Aryl Halide Using a Recyclable Fe(II)-Porphyrin Heterogeneous Photocatalyst

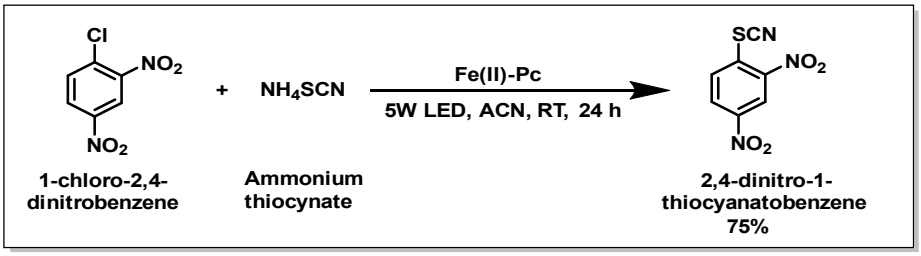
Kiran Vilas Butle, *Anurag Vinayak Pujari* and *Pundlik Rambhau Bhagat**

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

*Corresponding author: drprbhagat111@gmail.com, pundlik.rb@vit.ac.in (Pundlik Rambhau Bhagat)

Abstract: Developing sustainable methods for C–S bond formation remains an important objective in organic synthesis because aryl thiocyanates are versatile intermediates for pharmaceuticals, agrochemicals, and functional materials. In this work, a recyclable Fe(II)-porphyrin heterogeneous photocatalyst (Fe(II)-Pc) was achieved by coordinating ferrous sulfate with a sulfonic acid-functionalized porphyrin containing benzo-triazolium moiety. The photocatalytic performance of Fe(II)-Pc was evaluated for the thiocyanation of activated aryl halides under visible-light irradiation using ammonium thiocyanate (NH_4SCN) as the thiocyanate source. Under optimized conditions, 1-chloro-2,4-dinitrobenzene was converted into 2,4-dinitro-1-thiocyanatobenzene in acetonitrile under a 5 W LED at room temperature in 24 h. The catalyst promoted efficient C–S bond formation under mild reaction conditions without the use of harsh oxidants or elevated temperatures. These findings demonstrate that Fe(II)-Pc is a promising recyclable heterogeneous photocatalyst for visible-light-driven thiocyanation, offering a simple and environmentally friendly approach for the synthesis of aryl thiocyanates.

Scheme:



Scheme 1: Synthesis of 2,4-dinitro-1-thiocyanatobenzene

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PP-15

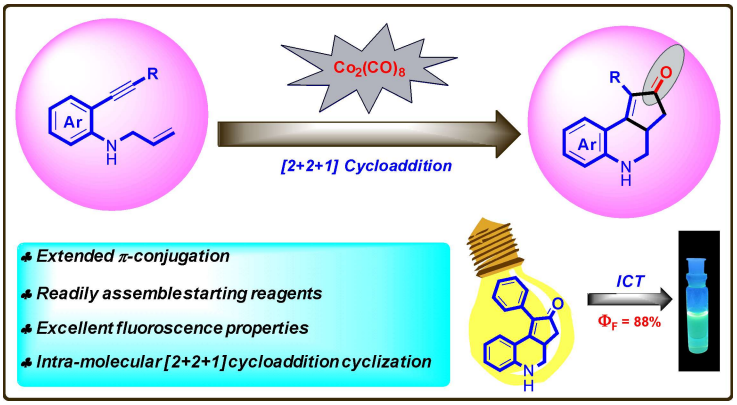
Cobalt-catalyzed Pauson–Khand synthesis of π-extended tetrahydrocyclopentaquinolinones: photophysical properties and DFT analysis

Ashutosh Dey,[a] Surendra Pothuraju,[b] Rohit Kumar Maurya,[a] Vikash Kumar,[a] Megha Kumari,[a] Kishor Padala,[c]* and Mahender Khatravath[a]*

Department of Chemistry, Central University of South Bihar, SH-7, Gaya Panchanpur Road, Karhara, Gaya-824236, Bihar, India;

E-mail: mkhatravath@cusb.ac.in; k.mahender666@gmail.com.

Abstract: Tetrahydrocyclopenta quinolinones, derived from tetrahydroquinoline, exhibit a wide range of biological activities, making them valuable scaffolds in medicinal chemistry.[1] These compounds are essential for developing new medications. They help combat tumors, fight infections, reduce inflammation, and relieve pain.[2] The π-extended tetrahydrocyclopenta quinolinones were effectively prepared using a Co-catalyzed Pauson-Khand reaction,[3] and their photophysical properties were examined. This protocol significantly creates complex quinolinone scaffolds, featuring the versatility and utility of transition metal catalysis. The compounds displayed a strong fluorescence quantum yield, and a comprehensive analysis of molecular structures like rigidity, coplanarity, and substituent effects explaind their impact on fluorescence efficiency. Density Functional Theory (DFT) calculations confirmed that extended π-conjugation and structural rigidity enhance radiative decay pathways. These insights into the relationship between molecular structure and photophysical behavior suggest future applications in material science, bioimaging, and photonic technology.



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PP-16

Microbial production of polyhydroxyalkanoates using *Bacillus sp.*: A sustainable approach toward bioplastic production

Dashrath Shriwas, *Rashmi Kataria**
Department of Bioscience and Technology (SBST)
Vellore Institute Of technology, Vellore
Tamil Nadu, India
*Corresponding author email: rashmi.kataria@vit.ac.in

Abstract: The growing accumulation of petroleum-based plastic waste has intensified the search for sustainable and biodegradable alternatives. Polyhydroxyalkanoates (PHA) are microbial polyesters which have been identified as potential candidates in the field of bioplastics owing to their biodegradability and biocompatibility.[12] The present study aims to evaluate PHA production by a bacterial isolate using glucose as the sole carbon source under submerged fermentation. Quantitative estimation of PHA is being carried out using the crotonic acid assay, while structural characterization is being performed through Fourier Transform Infrared (FTIR) spectroscopy and Gas Chromatography-Mass Spectrometry (GC-MS).[34] The study is designed to assess the suitability of glucose as an economical carbon source for microbial PHA production and to establish an effective extraction and characterization workflow. The findings are expected to contribute to the development of sustainable bioplastic production processes and support the application of biodegradable polymers as environmentally friendly alternatives to conventional plastics.

Keywords: Polyhydroxyalkanoates, Bioplastics, Glucose, Mineral Salt Medium, Sustainable Biotechnology, Microbial Fermentation

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PP-17

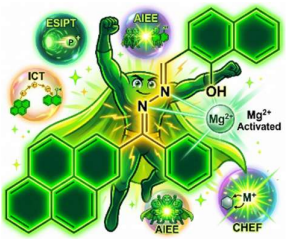
"When One Molecule Does It All: A Multi-Functional Fluorescent Probe with ESIPT, ICT, AIEE, and CHEF Mechanisms for Selective Mg^{2+} Sensing

Dineshkumar Arumugasamy and Sivakumar Shanmugam *
Department of Organic Chemistry,
School of Chemistry, Madurai Kamaraj University,
Madurai-625021.
Email: sivakumar.chemistry@mkuniversity.ac.in

Abstract: A new pyrene-naphthalene Schiff base probe (Py-Na-SB) was synthesized in a single step and characterized using NMR, Mass and UV-Vis/fluorescence spectroscopy. Remarkably, this one molecule combines four distinct photophysical behaviours: Excited-State Intramolecular Proton Transfer (ESIPT), Internal Charge Cransfer (ICT), Aggregation-Induced Emission Enhancement (AIEE), and metal-triggered fluorescence enhancement (CHEF). The probe shows bright solid-state emission, with its quantum yield increasing nearly 14-fold upon aggregation compared to solution. Among 18 metal ions tested, Py-Na-SB selectively and sensitively detects Mg^{2+}, forming a 1:1 complex with a detection limit of 2.40 μM. Fluorescence lifetime measurements show the probe becomes more rigid upon binding Mg^{2+}, explaining the enhanced emission. Computational (TD-DFT) studies further support the proposed ESIPT mechanism and confirm a significant increase in molecular polarity upon excitation, consistent with the observed large Stokes shift. This work presents a rare example of a single fluorophore integrating multiple emission mechanisms, offering a promising design strategy for next-generation selective ion sensors.

Keywords: : ESIPT; ICT; AIEE; CHEF; pyrene; Schiff base; TD-DFT

Figure/Scheme:



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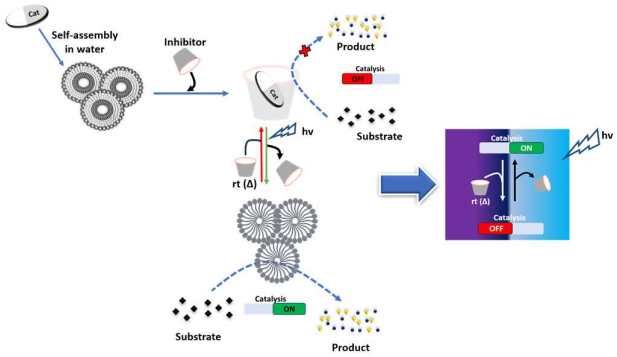
PP-18

Organocatalysis ON Demand: Light-Switchable Supramolecular Assemblies for Enzyme-Mimetic Aqueous Catalysis

*Divya Chauhan, Chandan Maity**
(Organic)Material Science & Engineering Lab, Department of Chemistry, Centre for Nanobiotechnology (CNBT), Vellore Institute of Technology (VIT), Vellore campus, Tamil Nadu, India – 632014
Email: divya.lalbhadur2023@vitstudent.ac.in

Abstract: Nature achieves adaptive functionality through the bottom-up assembly of simple molecular building blocks. Light-responsive supramolecular systems provide a powerful strategy for achieving remote, waste-free, and spatiotemporally precise control over function.[1,2] In this presentation, I will demonstrate how a minimalistic, light-switchable supramolecular organocatalytic platform enables reversible and spatiotemporally precise control of enzyme-mimetic activity in aqueous media.[3] The system integrates a photoresponsive molecular switch with a catalytically active unit, allowing light-directed modulation of supramolecular assembly and catalytic function. In the dark, the molecule self-assembles into vesicular nanostructures, whereas light irradiation triggers a vesicle → micelle transition, resulting in enhanced catalytic activity. Host–guest complexation with cyclodextrin acts as a molecular gatekeeper, suppressing catalysis under dark conditions and restoring activity upon irradiation. Thermal back-reaction enables fully reversible ON↔OFF catalytic switching with precise temporal control. The system exhibits hydrolase-like activity and follows Michaelis–Menten kinetics, demonstrating light-controlled modulation of catalytic rates. This strategy establishes a versatile framework for environmentally friendly, remotely controlled supramolecular catalysis and offers new opportunities in biomimetic chemistry and adaptive functional materials.



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PP-19

Design and Synthesis of Metal-free Organic Photosensitizer Molecules for Dye-Sensitized Solar Cells

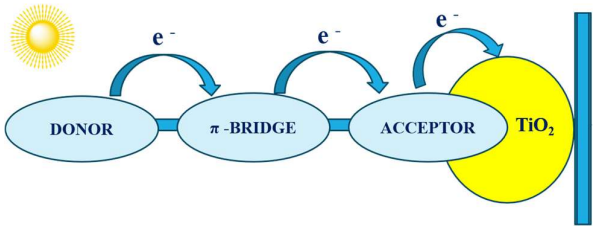
*Gayathri Y, Manju S L**

Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, Tamil Nadu, India

Email: slmanju@vit.ac.in

Abstract: Dye-sensitized solar cells (DSSCs) have emerged as promising alternatives to conventional silicon-based photovoltaics owing to their low cost, facile fabrication, and potential for sustainable solar energy conversion. The power conversion efficiency (PCE) of DSSCs strongly depends on the molecular structure and photophysical properties of the sensitizer. Metal-free organic dyes containing heterocyclic and π-conjugated units have attracted considerable interest because of their structural versatility and tunable optical and electronic properties. In this work, novel organic photosensitizers based on a donor–π–acceptor (D–π–A) architecture were designed and synthesized for potential application in DSSCs. Electron-rich donor moieties, including triphenylamine, carbazole, and indole, were integrated with π-conjugated spacers and cyanoacrylic acid as the electron-accepting and anchoring unit. Structural modification of the donor and π-spacer components was employed to promote intramolecular charge transfer, broaden visible-light absorption, and enhance light harvesting, which are important factors influencing PCE. The synthesized compounds were structurally characterized, and their photophysical properties were investigated using spectroscopic techniques. The sensitizers will subsequently be evaluated through electrochemical studies and DSSC fabrication to determine their photovoltaic characteristics and PCE. This work provides a molecular design strategy for developing efficient metal-free organic sensitizers with potential for enhanced DSSC performance and PCE.

Keywords: *D-π-A systems, heterocyclic units, photosensitizers, dye-sensitized solar cells (DSSCs), photovoltaic performance, Power*



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PP-20

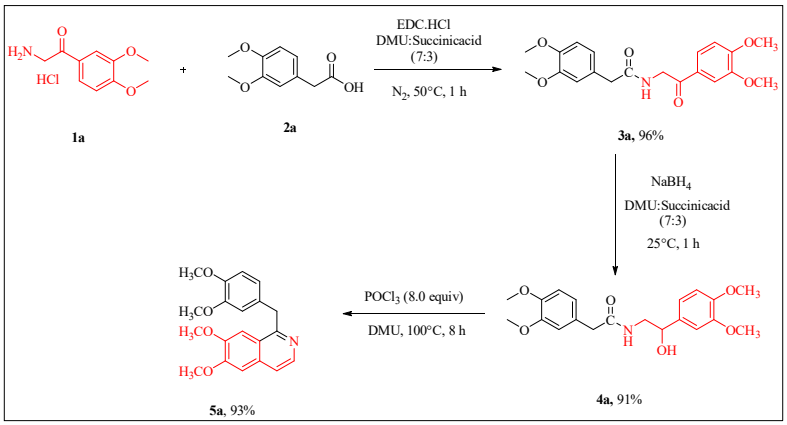
Synthesis and Late-Stage C–H Functionalization of Papaverines

*Saurabh B. Avachar, Sundararajan Suresh, Gollangi Madhusudanarao, Mathavan M, and Nawaz Khan F**

*Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India; *nawaz_f@yahoo.co.in*

Abstract: Papaverine is a pharmacologically valuable benzylisoquinoline alkaloid; however, its preparation and functionalization typically rely on volatile organic solvents, expensive catalysts, and harsh reaction conditions. This work presents a sustainable, stepwise synthesis of papaverine alongside its nickel-catalyzed late-stage benzylic C(sp^3)–H functionalization, carried out without volatile organic solvents during the reaction stages. A deep eutectic solvent (DES) made up of 1,3-dimethylurea and succinic acid (7:3) was used to facilitate the EDC-mediated coupling and $NaBH_4$ reduction steps, giving the corresponding amide and amino alcohol intermediates in 96% and 91% yields, respectively. A subsequent $POCl_3$-mediated Pictet–Spengler cyclization performed in 1,3-dimethylurea then delivered papaverine in 93% yield. Late-stage coupling of papaverine with substituted benzyl alcohols was carried out using $NiCl_2 \cdot 6H_2O$ (5 mol%), 1,10-phenanthroline (10 mol%), KO^{t}Bu (1.2 equiv.), and the DES at 100 °C for 7 h under nitrogen. This approach afforded thirteen functionalized papaverine derivatives in yields ranging from 75 to 89%, with electron-withdrawing substituents generally producing better results. The structure of representative derivative 7i was confirmed through single-crystal X-ray diffraction (CCDC 2374249). Control experiments and ^{1}H NMR studies support a mechanism involving alcohol dehydrogenation to an aldehyde, DES-assisted tautomerization of papaverine to an enamine, C–C bond formation, and dehydration. The scalability of this approach was demonstrated by preparing 3.62 g of papaverine in 92% yield and 1.87 g of derivative 7i in 81% yield. The derivatives showed emission between 389 and 471 nm, and selected compounds displayed positive solvatochromism. Overall, this methodology brings together sustainable synthesis, scalable API functionalization, and useful photophysical properties, making it relevant to both medicinal and materials chemistry applications.

Scheme - Total synthesis of papaverine



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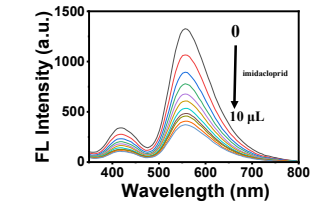
PP-21

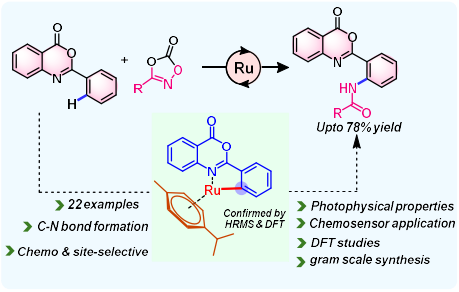
Ruthenium-catalysed site-selective C-H amidation of 2-arylbenzoxazinone using dioxazolone: DFT studies and fluorescence chemosensors for pesticide detection

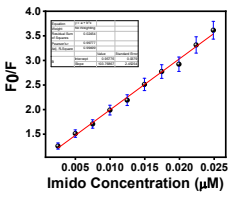
Krishnamoorthy Hariprasath, *Annamalai Pratheepkumar**
Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu 632014, India
hariprasath.tk2023@vitstudent.ac.in, pratheepkumar.a@vit.ac.in

Abstract: Herein we report a ruthenium-catalysed chemo- and site-selective C-H amidation of 2-arylbenzoxazinones using bench-stable dioxazolones as amidating agents. The transformation proceeds under mild reaction conditions with broad substrate scope and excellent functional-group tolerance, giving the desired amidated products in good to excellent yields. Density functional theory (DFT) studies were carried out to elucidate the reaction mechanism and rationalise the observed site-selectivity, revealing the preferential formation of a thermodynamically favourable ruthenacyclic intermediate. Also, the photophysical properties of the synthesised amidated benzoxazinone derivatives were studied. One representative derivative exhibited excellent fluorescence behaviour and high selectivity towards the pesticide imidacloprid, proving its potential as a fluorescent chemosensor. This work represents a combination of transition metal-catalysed C–H functionalization, mechanistic insight from DFT calculations and fluorescence sensing. It also provides an efficient approach for the synthesis of functional benzoxazinone derivatives with potential applications in environmental monitoring and chemical sensing.



Fluorescence spectra of 3p ($1.0 * 10^{-5}$ mol L^{-1}) in the presence of various concentrations of imidacloprid





Stern–Volmer plot based on the relative fluorescence signal [F0/F] and imidacloprid concentrations.

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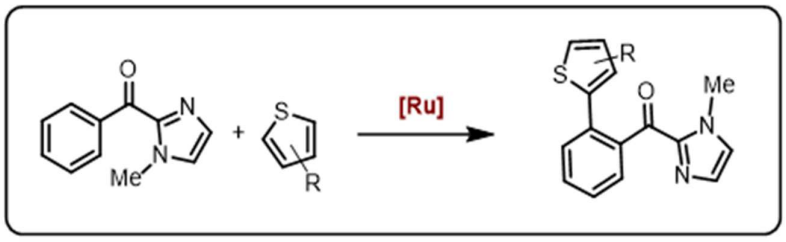
PP-22

Ru(II)-Catalysed Cross-Dehydrogenative Coupling of *C*-Acyl Imidazole with Thiophenes

*Jagathiswaran sargunam, Alagumalai Ramkumar, Thirumanavelan Gandhi**
Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, Tamil Nadu, India.
*E-Mail: velan.g@vit.ac.in, jagathiswaran.s2024@vitstudent.ac.in.

Abstract: A Ru(II)-catalyzed Cross-Dehydrogenative coupling (CDC) of *C*-Acyl imidazole with thiophenes has been developed for the direct construction of C–C bonds *via* C–H activation. The reaction undergoes smoothly without pre-functionalized substrates like organohalides and imidazolium salts, with excellent step economy and atom efficiency. Either imidazole moiety or carbonyl unit serves as an effective directing group, enabling regioselective arylation. The control studies are underway to ascertain the whether O or N atom acts the directing group. All the compounds were confirmed by ^{1}H and ^{13}C NMR spectroscopy. The method provides access to functionalized *C*-acyl imidazole derivatives of potential pharmaceutical relevance. This study demonstrates a sustainable approach to heteroaromatic C–H activation and functionalization.

Scheme:



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PP-23

Porphyrin-Based Catalysts for Sustainable Visible-Light-Assisted Knoevenagel Condensation

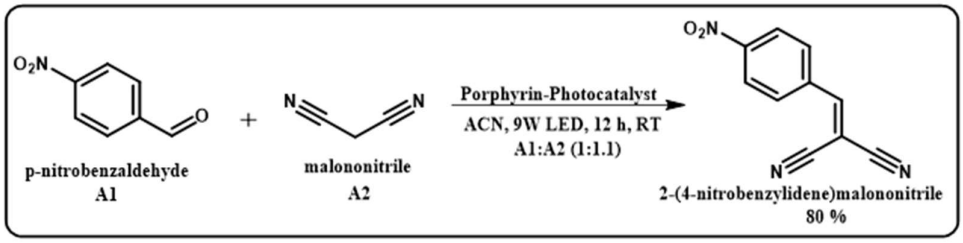
Rushikesh Rajaram Nigade[a], *Kaartik Kalpesh Chandan*[a] and *Dr. Pundlik Rambhau Bhagat*[a]*

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

* Corresponding author: drprbhagat111@gmail.com, pundlik.rb@vit.ac.in (Pundlik Rambhau Bhagat)

Abstract: In the present study, a porphyrin-based photocatalyst was acquired from 1-(4-formylphenyl)-3-sulfo-1H-benzo[d][1,2,3] triazol-3-ium chloride and pyrrole in acetic acid under reflux conditions. The synthesized photocatalyst was confirmed by using various analytical techniques for structural and physicochemical properties. The photocatalytic performance of the synthesized porphyrin was investigated for the Knoevenagel condensation of aryl aldehydes with active methylene compounds. The protocol represents a versatile and efficient synthetic strategy for construction of C=C bonds to acquire synthetically important alkene derivatives. In this work, the porphyrin photocatalyst was employed under low-power visible-light irradiation (9 W) at room temperature to afford Knoevenagel condensation under mild reaction conditions. The desired alkene product was obtained in good yield of 80% after 12 h of irradiation. The desired product was characterized by proton NMR and GC-MS spectra. Accordingly, the potential of porphyrin-based photocatalyst proved as an environmentally benign approach to the Knoevenagel condensation under visible-light irradiation.

Scheme:



Scheme 1. Synthesis of 2-(4-nitrobenzylidene)malnonitrile

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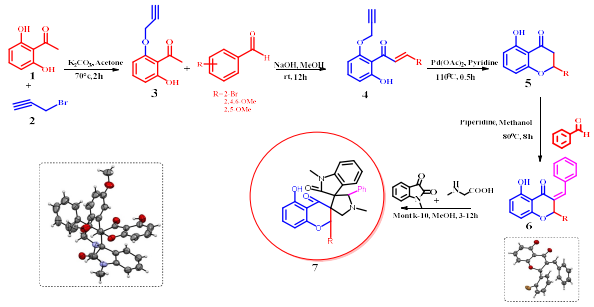
PP-24

Synthesis of Fused Heterocycles via [3+2] Cycloaddition of Alkylidene Flavanones with Azomethine Ylides

V. Kanmani*, *Jubin Chacko, K.R Ethiraj*

Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632 014, Tamil Nadu, India, Email: kethiraj.@vit.ac.in

Abstract: Alkylidenes are valuable precursors for synthesizing cycloaddition products. In these alkylidene compounds, the carbon-heteroatom double bond exhibits a polarized nature, where the carbon bears a partial positive charge and the heteroatom carries a partial negative charge. This polarization enables alkylidenes to efficiently undergo addition reactions and form cycloaddition products[1]. Alkylidene-based derivatives have attracted considerable interest in recent years due to their pronounced biological activities, particularly in anticancer and anti-inflammatory applications[2]. A multistep synthetic route was established beginning with the *O*-propargylation of 2,6-dihydroxyacetophenone, followed by Claisen–Schmidt condensation to afford *O*-propargylated chalcones. Subsequent depropargylation yielded flavanones, which were condensed with various aldehydes to give alkylidene flavanones. The resulting compounds underwent [3+2] cycloaddition with azomethine ylides to form fused heterocycles. Based on the results, the scope of the reaction was explored by synthesizing a series of cycloaddition products from respective alkylidenes. All the synthesized compounds were characterized by spectroscopic methods such as FTIR, ^{1}H NMR,^{13}C NMR, and HRMS. This study presents an efficient synthetic approach for generating structurally diverse fused heterocycles from alkylidene-substituted flavanones, offering a valuable platform for further structural modification and potential biological investigation.



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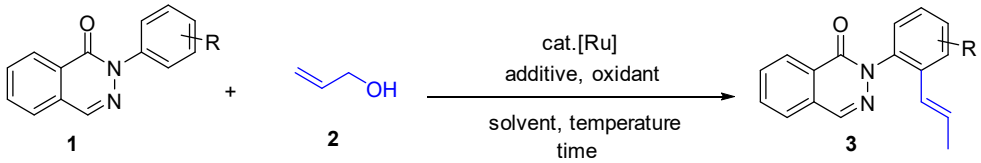
PP-25

Harnessing Allyl Alcohols as Vinylating Reagent: A Ru(II)-Catalysed Strategy for *Ortho*-Selective C–H Vinylation of bicyclic azaamide

*Karthick Raja Periyasamy, Alagumalai Ramkumar, Thirumanavelan Gandhi**
Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, Tamil Nadu, India.
*E-Mail: Velan.g@vit.ac.in, karthickraja.p2024@vitstudent.ac.in.

Abstract: Phthalazinones are privileged bicyclic aza-amide scaffolds exhibiting diverse biological and pharmaceutical activities. Direct C−H functionalization of these scaffolds provides an efficient route to structural diversification. Allyl alcohols are inexpensive and readily available C3 synthons; however, their application as vinylating reagents is unexplored due to its challenging *β*-hydroxy elimination. Herein, we developed a Ru(II)-catalyzed stereoselective C−H vinylation of *N*-aryl phthalazinones using allyl alcohol *via* C−H allylation followed by alkene isomerization. This protocol elucidates the atom-economical approach for the synthesis of valuable vinylated phthalazinone derivatives.

Scheme:



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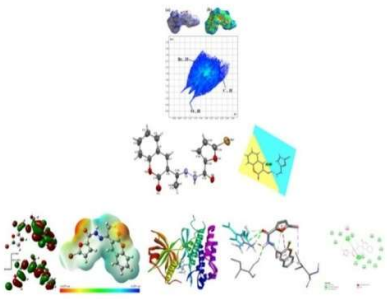
PP-26

Synthesis, crystal structure, quantum computational analysis and in-silico evaluation of 5-bromo-*N*′-(1-(2-oxo-2*H*-chromen-3-yl)ethyl)furan-2-carbohydrazide

Krishna Murthy S M [a b], *Chethan Prathap K N* [b],*
[a] Department of PG Studies in Physics, Government Science College, Chitradurga-577501, India.krishnamurthy.smk@gmail.com
[b] Department of Studies in Physics, University College Science, Tumkur University, Tumakuru, 570103, India. krishnamurthy.smk@gmail.com

Abstract: Coumarin derivatives are recognized as privileged scaffolds owing to their wide range of tic potential. In this study, the title compound, 5-bromo-N′-(1-(2-oxo-2H-chromen-3-yl)ethyl)furan-2-carbohydrazide**,** was synthesized via a nucleophilic substitution reaction. The molecular structure was confirmed by single-crystal X-ray diffraction analysis. The compound crystallizes in the triclinic crystal system with the space group *P-1* and is stabilized by intramolecular C–H···N interactions along with supramolecular synthons. Hirshfeld surface analysis revealed that O···H, H···H, and Br···H contacts are the predominant intermolecular interactions, emphasizing the contribution of hydrogen bonding and halogen contacts to crystal packing stability. Density functional theory (B3LYP/6-311+G(d, p)) calculations showed a HOMO–LUMO energy gap of 3.893 eV, indicating a favorable balance between molecular stability and chemical reactivity. Molecular docking studies against VEGFR-2 demonstrated strong hydrogen-bonding and hydrophobic interactions, suggesting potential inhibitory activity associated with angiogenesis. Collectively, the crystallographic, computational, and docking results highlight the compound as a promising candidate for future drug-design applications.



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PP-27

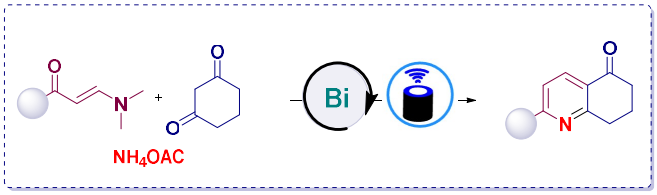
Visible-Light Promoted Synthesis of Dihydroquinoline Catalysed by Heterogeneous Nitrogen-Doped Bismuth Tungstate

Lambodar Khadanga[a], Selvaraj Mohana Roopan*

[a]Chemistry of Heterocycles and Natural Product Research Laboratory, Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu 632 014, India.

*Correspondence: mohanaroopan.s@vit.ac.in; Tel.: +91-0416-220-2313

Abstract: The dihydroquinoline is recognised as an important skeleton in drug innovation due to its intrinsic biological attributes. The dihydroquinolinone nucleus serves as a versatile pharmacophore for various biologically active molecules. From green chemistry perspective, utilising water as a solvent in photochemical synthesis provides a synthetic route for chemical transformations under mild conditions. Herein, we illustrate a simple and cost-effective visible-light-assisted protocol for dihydroquinoline synthesis utilising heterogeneous N-doped Bi_2WO_6 as a catalyst. The method is excellently compatible with functional groups and offers scalability for the dihydroquinoline product. Also, its practical utility for pharmaceutical development is viable. The post-synthetic transformations demonstrate the versatility of both the catalyst and the synthesized dihydroquinoline moieties.



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PP-28

Development of Mucilage /Poly (Ethylene Glycol) Composite Patches Containing Glycine Max Protein: Physiochemical Characterization and Biological Evaluation

Maithili Gurumoorthi [a], Nandhini R[b], Shiromi P[b], Meenatchi U[d], Jayanthi Abraham[d]*, Sasikumar Swamiappan*

[a] *Department of Chemistry, Centre for Clean Environment, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India*

Abstract: Skin wounds can occur when natural skin is damaged due to injury, burns, infections, diseases or surgery. It is generally classified in four types, which are acute wound, chronic wound, superficial wound and deep thickness wound. It is crucial to establish a biocompatible patch that prevents from infections and facilitates the skin tissue repair process. For skin tissue applications, multiple synthetic and natural polymers and composites were used, such as polyvinyl alcohol, sodium alginate, chitin, chitosan, gelatine, polylactic acid and hyaluronic acid. Improved wound dressings have been developed to address the limitations are limited bioactivity, inadequate antimicrobial performance, insufficient antioxidant properties and anti-inflammatory properties. Even though PEG and mucilage-based composites have been widely studied for wound dressing applications. The incorporation of extracted plant sourced protein composites limited. The present study aimed to fabricate mucilage/PEG composite patches incorporated with Glycine max protein and to examine their physicochemical properties and biological properties using XRD, FT-IR, SEM, stereo microscopy, antimicrobial, antioxidants and anti-inflammatory and hemolysis assays to assess their capability for wound healing applications.

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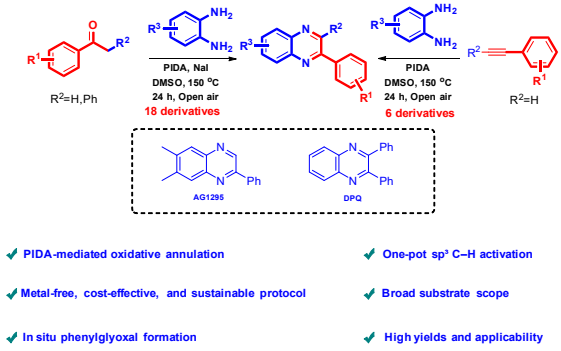
PP-29

Efficient Synthesis of Quinoxaline Derivatives *via* PIDA-Promoted Oxidative Annulation

Megha Kumari,[a] Ashutosh Dey,[a] Vikash Kumar,[a] Rohit Kumar Maurya,[a,b] Kishor Padala,[c] and Mahender Khatravath*[a]*

[a]*Department of Chemistry, Central University of South Bihar, SH-7, Gaya Panchanpur Road, Karhara, Gaya-824236, Bihar, India; E-mail: mkhatravath@cusb.ac.in; k.mahender666@gmail.com,*
[b]*Chemveda Life Sciences, Mallapur, Hyderabad, Telangana, 500076, India*
[c]*Department of Chemistry, Central Tribal University of Andhra Pradesh, Vizianagaram, Andhra Pradesh-53003, India, E-mail: kishor.padala@gmail.com; kishor.padala@ctuap.ac.in.*

Abstract: Quinoxaline derivatives represent an important class of privileged heterocyclic scaffolds widely present in natural products and biologically active molecules.[1] Herein, we report a novel and efficient oxidative annulation strategy for the synthesis of quinoxalines *via* Phenyliodine diacetate[2] (PIDA)-mediated transformation of acetophenones/ phenyl acetylene derivatives with 1,2-diamines. This protocol utilizes inexpensive and readily available starting materials and proceeds through in situ formation of phenyl glyoxal, followed by condensation and subsequent aromatization. The method exhibits broad functional group tolerance and delivers the desired quinoxaline derivatives in high yields. Notably, the combination of PIDA and NaI serves as a metal-free and cost-effective oxidizing system, highlighting the practicality and sustainability of the approach. Furthermore, this methodology enables the synthesis of biologically active compounds such as AG 1295, a PDGFR inhibitor that suppresses cell proliferation, and DPQ[3], a PARP inhibitor that disrupts DNA repair and induces cell death. Overall, the synthesized quinoxalines serve as valuable intermediates with promising applications in natural product synthesis and medicinal chemistry.



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PP-30

Sustainable Synthesis of Fused Chromenoquinolines: A Route to Emerging Functional Materials

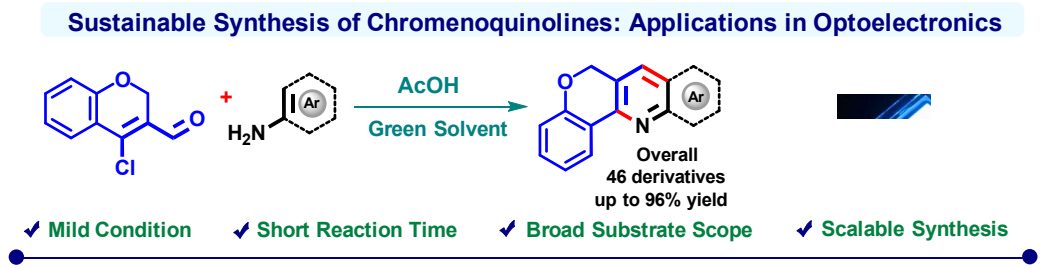
Paranimuthu Panjacharam,[a] *Jwo-Huei Jou,*[b] Sabbasani Rajasekhara Reddy*[a]*

[a]School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014, India.

[b]Department of Materials Science & Engineering, National Tsing Hua University, Hsinchu, Taiwan.

E-mail: paranipanjachram@gmail.com, sekharareddy@vit.ac.in, jjou@mx.nthu.edu.tw

Abstract: A metal- and oxidant-free synthesis of diverse 6*H*-chromeno[4,3-*b*]quinolines from β-chlorovinyl aldehydes was developed *via* an acetic acid-promoted Doebner–Von Miller-type reaction. The protocol efficiently couples substituted anilines with 4-chloro-2*H*-chromene-3-carbaldehydes, enabling C–N and C–C bond formation with simultaneous construction of the fused heterocyclic framework. The method provides versatile chromenoquinoline scaffolds for subsequent cross-coupling reactions and C(sp3)–H oxidation. The synthesized derivatives were further evaluated through photophysical studies and DFT calculations, revealing promising emission properties and favourable electronic characteristics for potential optoelectronic applications.



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PP-31

Catalyst-Assisted Green Synthesis of Novel Azo-Fused Tetrahydro-1*H*-Xanthenyl-5,5-Dimethylcyclohexane-1,3-Dione Derivatives: Integrating Antimicrobial Evaluation and Computational Insights

Udhayakumar Peroli[a] and Appaswami Lalitha[a,*]
[a]*Department of Chemistry, Periyar University, Salem-636011, Tamil Nadu, India.*
lalitha2531@yahoo.co.in, Tel: +91-427-234-5271; Fax: +91-427-234-5124.

Abstract: Catalyst-assisted synthesis has emerged as an efficient strategy for the rapid construction of biologically important heterocyclic compounds while promoting sustainable and environmentally friendly chemical processes. In the present study, a simple, efficient and green one-pot two-component protocol was developed for the synthesis of a series of azo fused tetrahydro-1*H*-xanthenyl-5,5-dimethylcyclohexane-1,3-dione derivatives using Amberlyst® A21, a recyclable heterogeneous base catalyst, in ethanol as a green solvent. The reaction between arylazo aldehydes and dimedone under reflux conditions afforded the desired products in excellent yields with shorter reaction times, simple work-up procedures and broad functional group compatibility. The synthesized compounds were comprehensively characterized by FT-IR, ^{1}H NMR, ^{13}C NMR, ESI-MS spectroscopy and SC-XRD.

To elucidate the molecular interactions of their biological activity, molecular docking studies were performed to evaluate the binding interactions with the target protein. The biological potential of the synthesized derivatives was investigated through antimicrobial activity studies, which identified promising lead compounds with enhanced inhibitory activity against selected microbial strains. The integration of green synthesis, biological evaluation and computational studies demonstrates the potential of these derivatives as promising candidates for the development of new bioactive agents.

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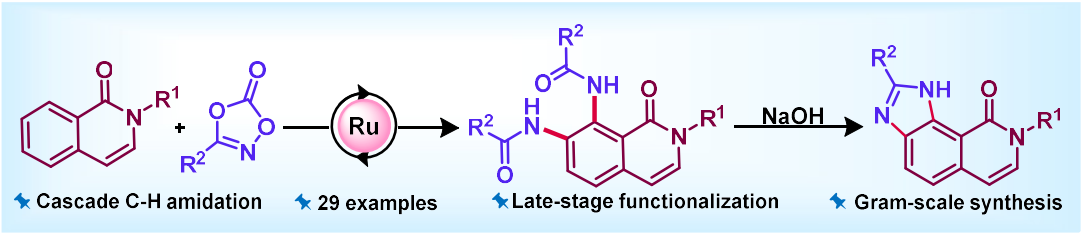
PP-32

Ru(II)-catalyzed cascade regioselective C-7 and C-8 diamidation of isoquinolinones using dioxazolones

Ravichandran Manikandan and Annamalai Pratheepkumar*
Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu, India - 632 014
Email: manikandan.r2019@vitstudent.ac.in and pratheepkumar.a@vit.ac.in

Abstract: In this study, we disclose an unprecedented ruthenium-catalyzed selective C-7 and C-8 diamidation of isoquinolinones *via* weak chelation assistance, employing dioxazolones as an efficient amidating agent. Significantly, in this reaction, dual C-H bonds were functionalized in one pot, enabling isoquinolinones embedded in diamidated scaffolds with high efficiency. The developed protocol enables the efficient synthesis of a broad array of diamidated isoquinolinones derivativities in excellent yields, including pharmaceutically relevant motifs derived from carboxylic acid and fatty acid containing dioxazolones. The resulting products exhibit excellent compatibility towards further synthetic diversification.



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PP-33

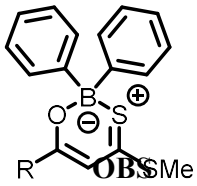
Design and synthesis of thio-ketonate (*OS*) boron complex and its photophysical studies.

Pandi Vijayan and Sivakumar Shanmugam *
Department of Organic Chemistry,
School of Chemistry, Madurai Kamaraj University,
Madurai-625021.
Email: sivakumar.chemistry@mkuniversity.ac.in

Abstract: The thio-ketonate boron complex was designed and synthesized. This study focused on the selective synthesis of thio-ketonate boron complex (OBS) from readily available starting material such as β-thioketnate and phenylboronic acid in moderate to good yields. The characteristic features of this methodology include operational simplicity, metal-free reaction conditions, gram-scale scalability, broad functional group tolerance, and short reaction times. There has been recent progress in creating four-coordinate boron complexes with emissions spanning from blue to red. These complexes show dazzling fluorescence in the solid state. Despite these advances, red-emitting organoboron compounds in the solid state remain relatively rare.

Keywords: β-thioketnate, phenylboronic acid, Organoboron,

Figure/Scheme:



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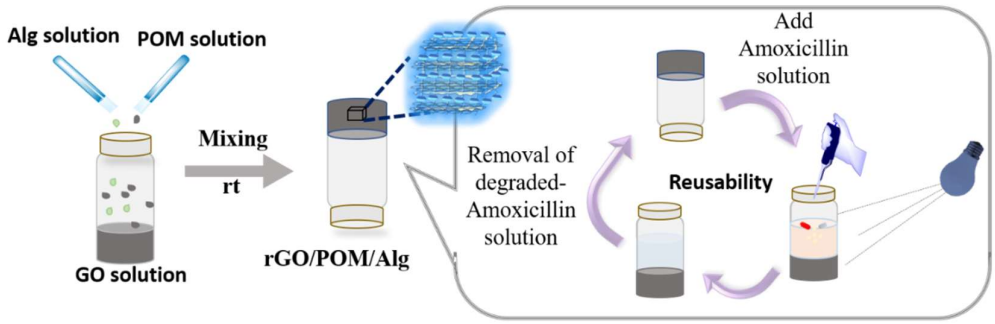
PP-34

From Solution to Purification: In-Situ Formation of rGO/POM–Alginate Hydrogels for Photocatalytic Amoxicillin Removal

*Devi Lakshmi Saravanan, Dr. Chandan Maity**
(Organic)Material Science and Engineering Laboratory, Department of Chemistry, School of Advanced Sciences (SAS), Centre for Nanobiotechnology (CNBT), Vellore Institute of Technology (VIT), Vellore Campus, Tamil Nadu-632014, India.
Email: chandanmaitylab@gmail.com, chandan.maity@vit.ac.in

Abstract: The increasing occurrence of pharmaceutical contaminants such as amoxicillin in aquatic environments necessitates efficient and sustainable remediation strategies. Graphene-based materials offer considerable potential for photocatalytic water treatment.[1] However, their preparation and integration into hybrid materials often require high-temperature processing, multiple synthesis steps, and specialized equipment. Herein, I will present how a solution-mixing strategy enables in-situ formation of reduced graphene oxide (rGO) within a polyoxometalate (POM)-integrated alginate hydrogel (rGO/POM/Alg) under ambient conditions.[2] This approach enables simultaneous rGO formation and hydrogel network development, eliminating separate rGO synthesis and high-temperature treatment. The resulting rGO/POM/Alg hydrogel exhibited efficient light-induced degradation of amoxicillin in aqueous media and maintained its photocatalytic activity over 15 consecutive cycles, demonstrating good reusability and operational stability.[3] Overall, this study presents a simple, energy-efficient, and environmentally friendly approach for constructing reusable rGO/POM/Alg hydrogel photocatalysts, offering a promising platform for sustainable water purification and remediation of pharmaceutical-contaminated water.



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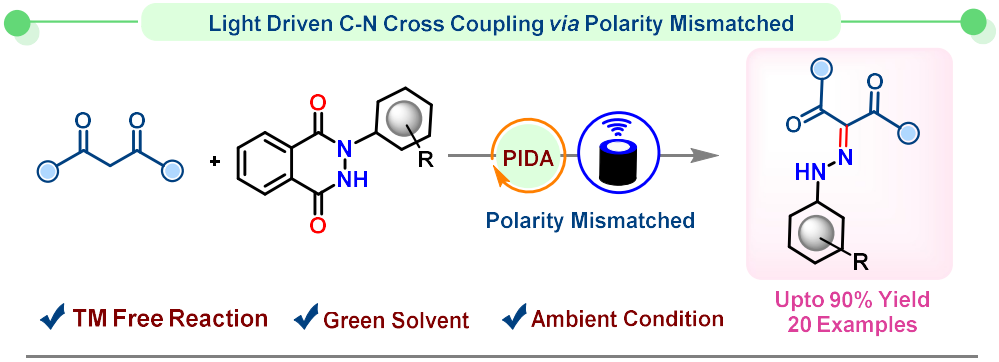
PP-35

Photochemical *in situ* Generation of Nitrenes and Carbenes for Polarity-Mismatched C−N bond Cross-Coupling

Sabariraja Jothimani,[a] Saravana Bhava S.,[a] Chandrasekaran Sivaraj[b] and Thirumanavelan Gandhi[a]*
[a]*Vellore Institute of Technology, Vellore 632014,* [b]*University of Valencia, Spain.*
Email: sabariraja172002@gmail.com, saravanaoffical21@gmail.com, sivarajchandrasekaran97@gmail.com and velan.g@vit.ac.in

Abstract: The formation of the Carbon-Nitrogen bond is a cornerstone of organic synthesis and its play a vital role in the drug synthesis, yet its development remains constrained by inherent polarity-matching requirements. Polarity-Mismatched cross-electrophile coupling (XEC)[1] has recently emerged as a powerful platform for forging C–X bonds through the direct union of two electrophilic partners and its having high selective product formation.[2-4] Herein, we disclose a blue LED-mediated hypervalent iodine strategy that enables the *in situ* generation of nitrene and carbene electrophilic intermediates under ambient conditions, facilitating rapid and unusual polarity-mismatched cross-coupling for efficient C–N bond construction**.**



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PP-36

Ruthenium-supported ionic liquid-based periodic mesoporous organosilica catalyst for sp^3 C-H bond alkylation of *9H*-fluorene with primary alcohols

G. Satishkumar[a*] *and Amit. B. Soni*[a]

Advanced Materials and Catalysis Lab, Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, E-mail: satishkumar.g@vit.ac.in.

Abstract: Substituted monoalkylated fluorene derivatives are mainly found in pharmaceuticals, polymerization synthesis, plastics, and dye industries. Therefore, synthesis of monoalkylated fluorene derivatives is highly significant and desirable. In this work, periodic mesoporous organosilica (PMO) has been functionalized with the ionic liquid 1-methyl-3-(trimethoxysilylpropyl) imidazolium chloride by utilizing the alkoxy groups (-OR) located in the pore wall of PMO, which assist in the effective stabilization of Ru supported over PMO-IL. The textural, structural, and morphological properties of the catalyst were studied using various analytical techniques, including XRD, BET, TGA, FTIR, ^{29}Si(CP-MAS), ^{13}C(CP-MAS)-NMR, XPS, ICP-OES, FE-SEM, and HR-TEM. In this study, we present a green and efficient protocol for the synthesis of monoalkylated derivatives via sp^3 C-H bond functionalization of *9H*-fluorene with primary alcohol by adopting the borrowing hydrogen strategy, thereby excluding the use of toxic alkyl halides. The reaction was catalyzed by a minimal loading of Ru@PMO-IL (2.5 wt%), without the need for any ligands or an external hydrogen source. The resulting catalyst showed excellent catalytic activity, a high turnover number (TON), and a wide substrate scope, including substituted primary alcohols and substituted 9H-fluorene derivatives, affording the corresponding alkylated products in good to excellent yields. Furthermore, the catalyst was recycled for 5 catalytic cycles and showed negligible loss in catalytic activity.

PP-37

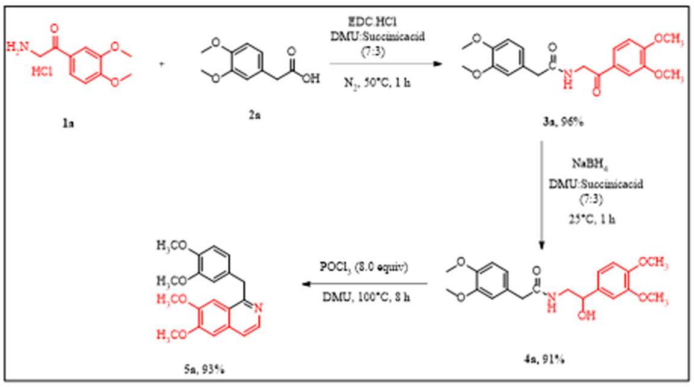
Synthesis and Late-Stage C–H Functionalization of Papaverines

*Saurabh B. Avachar, Sundararajan Suresh, Gollangi Madhusudanarao, Mathavan M, and Nawaz Khan F**

*Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India; *nawaz_f@yahoo.co.in*

Abstract: Papaverine is a pharmacologically valuable benzylisoquinoline alkaloid; however, its preparation and functionalization typically rely on volatile organic solvents, expensive catalysts, and harsh reaction conditions. This work presents a sustainable, stepwise synthesis of papaverine alongside its nickel-catalyzed late-stage benzylic C(sp^3)–H functionalization, carried out without volatile organic solvents during the reaction stages. A deep eutectic solvent (DES) made up of 1,3-dimethylurea and succinic acid (7:3) was used to facilitate the EDC-mediated coupling and $NaBH_4$ reduction steps, giving the corresponding amide and amino alcohol intermediates in 96% and 91% yields, respectively. A subsequent $POCl_3$-mediated Pictet–Spengler cyclization performed in 1,3-dimethylurea then delivered papaverine in 93% yield. Late-stage coupling of papaverine with substituted benzyl alcohols was carried out using $NiCl_2 \cdot 6H_2O$ (5 mol%), 1,10-phenanthroline (10 mol%), KO^{t}Bu (1.2 equiv.), and the DES at 100 °C for 7 h under nitrogen. This approach afforded thirteen functionalized papaverine derivatives in yields ranging from 75 to 89%, with electron-withdrawing substituents generally producing better results. The structure of representative derivative 7i was confirmed through single-crystal X-ray diffraction (CCDC 2374249). Control experiments and ^{1}H NMR studies support a mechanism involving alcohol dehydrogenation to an aldehyde, DES-assisted tautomerization of papaverine to an enamine, C–C bond formation, and dehydration. The scalability of this approach was demonstrated by preparing 3.62 g of papaverine in 92% yield and 1.87 g of derivative 7i in 81% yield. The derivatives showed emission between 389 and 471 nm, and selected compounds displayed positive solvatochromism. Overall, this methodology brings together sustainable synthesis, scalable API functionalization, and useful photophysical properties, making it relevant to both medicinal and materials chemistry applications.

Scheme - Total synthesis of papaverine



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PP-38

Visible-Light Heterogeneous Photocatalysis for the Redox Neutral Tandem Process to Synthesize Pyrazolo-Fused Heterocycles.

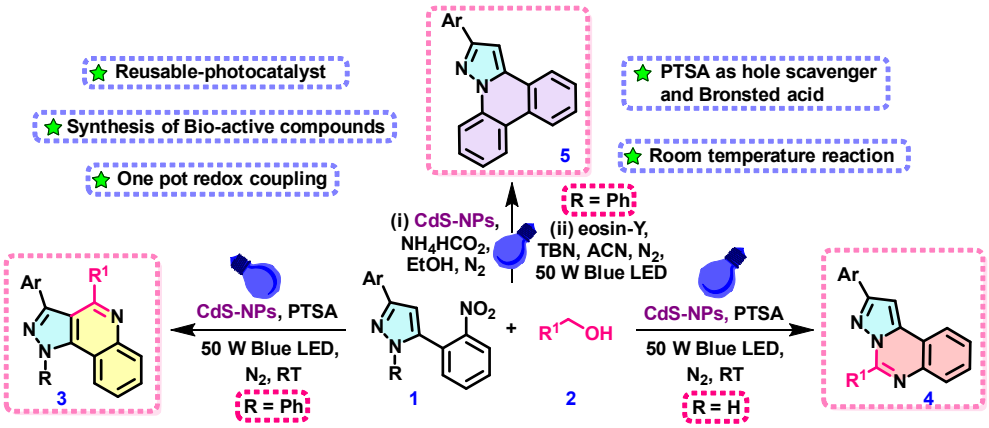
Markabandhu Shanthi[a], Koushikaa Selvapandian[a], Karuppaiah Perumal[a], Bhaskaran Shankar[b], Vijayakumar Hemamalini[a], Subburethinam Ramesh[a]*

[a]Department of Chemistry, School of Chemical and Biotechnology, SASTRA Deemed University, Thanjavur-613 401, Tamil Nadu, India. E-mail: rameshsbdu@gmail.com

[b]Department of Chemistry, Thiagarajar College of Engineering, Madurai 625 015, Tamil Nadu, India.

Abstract: Here we report an efficient and sustainable visible-light driven protocol for the synthesis of structurally diverse pyrazolo-fused heterocycles, including pyrazolo[4,3-c]quinoline and pyrazolo[1,5-c]quinazoline derivatives, under mild reaction conditions.[1] This methodology employs 50 W blue LED irradiation in the presence of cadmium sulfide nanoparticles (CdS-NPs) as photocatalyst, enabling a cascade transformation involving nitroarene reduction, alcohol oxidation and subsequent cyclization.[2] The developed protocol exhibits broad substrate scope, accommodating a wide range of aliphatic and aromatic alcohols, and delivers the desired products in good to excellent yields with high selectivity.[3,4] Notably, this strategy avoids the use of hazardous reagents and elevated temperature, offering an environmentally benign and operationally simple alternative to conventional methods.

Figure/Scheme:



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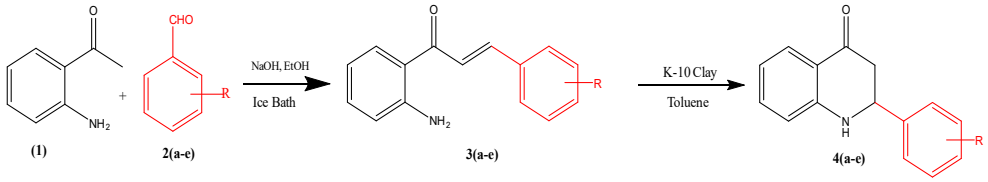
PP-39

Chalcone-Derived Aza-Flavones: Synthesis, Structural Characterization and In Silico ADME Profiling

*Ujjawal Sharma, Shubham Mazumdar, K. R. Ethiraj**
Department of Chemistry, Vellore Institute of Technology, Vellore – 632014, Tamil Nadu, India
krethiraj@vit.ac.in

Abstract: Flavones are an important class of flavonoids known for their diverse biological activities. Aza-flavones, a class of heterocyclic compounds structurally modified from the flavones, have gained considerable attention because of their anticancer, antimicrobial, antioxidant, anti-inflammatory, and enzyme inhibitory properties. In the present study, a small library of azachalcones was synthesized by the Claisen–Schmidt condensation of 2-aminoacetophenone with a series of heterocyclic aldehydes (**3(a-e)**), followed by cyclization under different reaction conditions to afford the corresponding aza-flavone derivatives. The synthesized compounds were assessed for their drug-likeness through in silico pharmacokinetic analysis, and all derivatives exhibited favourable molecular properties consistent with established drug-likeness criteria. These findings highlight the potential of the aza-flavone scaffold as a promising platform for the development of biologically active molecules. Future work will focus on optimizing the cyclization process to improve the conversion of azachalcones into aza-flavones and on further biological evaluation of the synthesized compounds to explore their therapeutic potential.

Figure/Scheme:



Scheme 1: Synthesis of Aza-flavones

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PP-40

Harnessing UV Light to Create Oxygen Vacancy-Enriched Black BiOCl for Enhanced Visible-Light Photocatalytic Degradation of Rhodamine-B.

Johan Oommen Cherian [1], *Steffy Mariyam Varghese* [1], *Akshay M Achari* [2], *Swati G* [2]*
[1] *Department of Chemistry, SAS, Vellore Institute of Technology, Vellore, 632014*
[2] *Centre for Nanotechnology Research (CNR), Vellore Institute of Technology, Vellore, 632014*
**swati.g@vit.ac.in*

Abstract: Bismuth oxychloride (BiOCl) is a potent semiconductor photocatalyst, but its wide band gap limits its efficacy under visible light[1]. This study demonstrates a novel approach using UV-induced defect engineering to create controlled oxygen vacancies, thereby enhancing BiOCl's visible-light activity. BiOCl was synthesized via a one-pot coprecipitation method. As obtained, pristine BiOCl was irradiated with UV-C (254 nm) light for various durations to examine the effects on its structural, optical, and photocatalytic properties. X-ray diffraction (XRD) confirmed that UV treatment maintained BiOCl's crystal structure, with modifications occurring at the surface. UV–Vis diffuse reflectance spectra showed increased absorption in the visible range, and photoluminescence (PL) studies revealed reduced charge recombination for the irradiated sample. Samples irradiated for 10 hours showed promising photocatalytic degradation of Rhodamine B. Further increasing the duration of irradiation reduced the performance due to the introduction of excessive oxygen vacancies that introduce recombination centres[2,3]. This research offers a straightforward and effective strategy for enhancing BiOCl through self-induced defect engineering, providing valuable insights into its photocatalytic mechanisms and promoting its application in environmental remediation.

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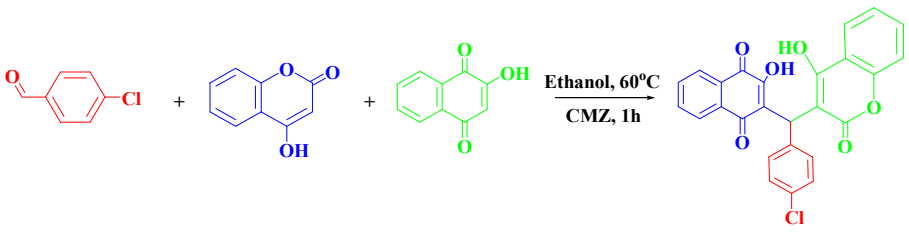
PP-41

Synergistically Enhanced Catalytic Activity of Ternary CeO_2-MoO_3-ZnO Nanocomposite Toward Bioactive Coumarin-Naphthoquinone Derivatives

Sumaiya Tabassum[1], *Santhosh G*[2]*
[1]*Department of Chemistry, Surana College - Autonomous, Bengaluru, 560004, India*
[2]*Department of Sciences and Humanities, Christ University, Bengaluru, 560074, India*
**Corresponding author: sumaiyatabassum2711@gmail.com*

Abstract: In line with the principles of sustainable and green chemistry, we fabricated a ternary CeO_2-MoO_3-ZnO (CMZ) nanocatalyst *via* a simple, eco-friendly co-precipitation method and evaluated it as an efficient heterogeneous catalyst for the one-pot synthesis of coumarin-naphthoquinone derivatives. Comprehensive characterisation by X-ray diffraction (XRD), scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDS), Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and transmission electron microscopy (TEM) confirmed the formation of a highly crystalline, thermally stable nanocomposite with a uniform particle size of 10-20 nm, characteristics favourable for sustainable catalytic applications. The CMZ nanocatalyst demonstrated strong green credentials in catalysing the three-component reaction of aromatic aldehydes, 4-hydroxycoumarin, and 2-hydroxy-1,4-naphthoquinone, achieving high yields (90-95%) in 1 hour under mild, environmentally benign conditions, without harsh solvents or prolonged heating. Beyond its catalytic efficiency, the protocol exemplifies key tenets of green chemistry, including atom economy, operational simplicity, and reduced environmental footprint, while avoiding hazardous reagents typically associated with conventional synthetic routes. Notably, the resulting coumarin-naphthoquinone derivatives exhibited promising antimicrobial activity, adding biological relevance to this environmentally conscious synthetic strategy. Collectively, these findings position the CMZ nanocatalyst as a sustainable and reusable catalytic platform for the eco-friendly construction of biologically important heterocyclic scaffolds, aligning with the broader goals of green and sustainable chemistry.

Figure/Scheme: Application of CMZ Nanocatalyst in organic synthesis



.PP-42

One-Pot, Multicomponent Cascade Synthesis of 3-Ketoquinolines from Terminal Alkynes and Anthranils Using DMSO as a Dual Synthon

Ajay Uppuluru, Kishor Padala[b]* Annamalai Pratheepkumar [a]*

[a]*School of Advanced Sciences, Vellore Institute of Technology, Katpadi, Vellore, Tamil Nadu, 632014, India. E-mail: pratheepkumar.a@vit.ac.in, kumarpratheep0@gmail.com*

[b]*Department of Chemistry, Central Tribal University of Andhra Pradesh, Vizianagaram, Andhra Pradesh, 535003, India. E-mail: kishor.padala@gmail.com, kishor.padala@ctuap.ac.in*

Abstract: A transition-metal-free one-pot three-component cascade strategy has been explored for the synthesis of 3-ketoquinolines from terminal alkynes and anthranils using DMSO as both solvent and a dual synthon. The transformation proceeds under $K_2S_2O_8$-mediated conditions *via* in *situ* generation of *α,β*-unsaturated ketone intermediates, followed by aza-Michael addition and intramolecular cyclization. This methodology offers broad substrate scope and excelllent functional group comatibility, affording a diverse range of 3-ketoquinolines in moderate to excellent yields. The operational simplicity, avoidance of transition metals, and the unique dual role of DMSO make this protocol an efficient and sustainable route to pharmaceutically relevant quinoline scaffolds.

Figure/Scheme:-

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PP-43

Extraction of lignin from agricultural waste by using green extraction method and its potential as an antimicrobial agent

*Vishal Kaushik, Rashmi Kataria**
School of Biosciences and Technology
Vellore institute of technology, Vellore, Tamil Nadu, India, 632014
Vishal.kaushik2023@vitstudent.ac.in
rashmi.kataria@vit.ac.in

Abstract: Lignocellulosic biomass is the most readily available renewable resource for production of sustainable products. In order to improve the ecological sustainability of the process of utilizing lignocellulosic biomass, a crucial lignin byproduct is given special consideration. Lignin has remarkable antibacterial properties because of its intricate phenolic polymer composition. In this research, agricultural waste was used as a lignocellulosic biomass as it is improperly disposed of, representing a large waste of natura resources. Deep eutectic solvent (DES) has been used to extract lignin from the agricultural waste. Agricultural waste was pretreated by using choline chloride as a hydrogen bond acceptor (HBA) and several carboxylic acids like lactic acid, acetic acid, formic acid and propionic acid as hydrogen bond donor (HBD) with different molar ratios at 120 ˚C and 150˚C. The black liquor obtained was mixed with an antisolvent to precipitate the lignin. This extracted lignin was further used to test the antimicrobial activity against various microbes by using agar well diffusion method. Zone of inhibition was observed and measured to know the antimicrobial ability of the extracted lignin.

Keywords: Agricultural waste, Lignin, Extraction, Deep Eutectic Solvent, Antimicrobial activity

PP-44

Exploring Marine Microorganisms as Sustainable Sources of Antimicrobial Metabolites

Yesasvini Muniraj[1], *Rohit Ruhal*[2]*, *Rashmi Kataria*[2]*

[1]*Center for Biomaterials, Cellular and Molecular Theranostics, Vellore Institute of Technology, Vellore, 632014, Tamil Nadu, India.*

[2]*School of Biosciences and Biotechnology, Vellore Institute of Technology, Vellore, 632014, Tamil Nadu, India.*

Email Id: Yesasvini.muniraj2024@vitstudent.ac.in, rohit.r@vit.ac.in, rashmi.kataria@vit.ac.in

Abstract:The global surge in antimicrobial resistance (AMR), combined with the stagnation of traditional antibiotic discovery pipelines, has intensified the search for novel bioactive compounds. Marine-derived bacteria and fungi, evolved under extreme physicochemical stresses such as temperature variations, hydrostatic pressure, high salinity and nutrient limitation, represent a prolific yet under-explored reservoir of structurally unique secondary metabolites. In this study, we isolated culturable microorganisms from seawater and marine sediment and evaluated their antibacterial potential against *Staphylococcus aureus* and *Pseudomonas aeruginosa* using disk diffusion antimicrobial assays, a subset of recovered isolates demonstrated clear zones of inhibition, providing preliminary evidence of their capacity to biosynthesize antibacterial metabolites. While these initial finding highlight the promising bioactivity of the isolates, this study provides a rigorous methodological roadmap for the next phase of drug discovery. These findings provide a baseline for future bioassay-guided purification and molecular identification, underscoring the potential of marine microbes to contribute to the next generation of sustainable antimicrobial therapeutics

Keywords: Marine microorganisms; Antimicrobial metabolites; Sustainable biotechnology; Marine biodiversity.

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PP-45

Upconversion Luminescence in Er^{3+} doped and Er^{3+}/Yb^{3+}-codoped $BiYWO_6$ Phosphor

Shubham Warudkar[1]†, Nilesh S. Ugemuge[1]†, Shruti P. Dhale[1,4]† Ashvini R. Pusdekar[1,2]†, R.V. Badre[3]

[1]*IHLR & SS, Department of Physics, Anand Niketan College, Anandwan, Warora 442907, India.*
[2]*Nano Materials and Device Laboratory, Department of Physics, Visvesvaraya National Institute of Technology, Nagpur, 440010, India.*
[3]*Department of Physics, Government Vidarbha Institute of Science and Humanities, Amravati 444604, India.*
[4]*G H Raisoni College of Engineering, Nagpur, 440016, India*
†Corresponding author's e-mail: nileshugemuge@gmail.com,

shubhamwarudkar112@gmail.com, shrutidhale@gmail.com (Shruti P. Dhale)
pusdekarashvini2407@gmail.com

Abstract: Lanthanide-doped upconversion phosphors have attracted considerable attention owing to their ability to convert low-energy near-infrared (NIR) radiation into higher-energy visible emission. In context of this, Er^{3+} and Er^{3+}/Yb^{3+} doped $BiYWO_6$ phosphor is synthesized by using solid state reaction (SSR) method and systematically investigated to understand their structural and upconversion luminescence properties. X-ray diffraction (XRD) analysis confirmed the formation of the crystalline $BiYWO_6$ phase, with the observed diffraction peaks in good agreement with the standard reference pattern. Average crystallite size of approximately 61.08 nm and microstrain of 53.2 $\times 10^{-4}$ is estimated from the W-H plot. The Raman spectra exhibited characteristic vibrational modes associated with the WO_6 group, confirming the structural integrity of the $BiYWO_6$ host lattice. SEM, EDS, and elemental mapping confirmed the formation of the synthesized material, revealing agglomerated morphology and a homogeneous distribution of Bi, Y, W, and O elements. Upconversion study revealed that the Yb^{3+} ions efficiently absorb NIR radiation due to their larger absorption cross-section at 980 nm, transferring that energy to Er^{3+} ions to obtain the upconversion emission in green and red region owing to the transitions $^2H11/2 \rightarrow {}^4I15/2$ (525 nm), $^4S3/2 \rightarrow {}^4I15/2$ (545 nm) and $^4F9/2 \rightarrow {}^4I15/2$ (654 nm) respectively, along with presence of various Stark components. On account of this study, the as-synthesized phosphors highlights the potential of for NIR-to-visible spectral conversion, optical sensing, and optical security applications.

Key Words: Photoluminescence; Upconversion; Phosphor; Er^{3+}, Er^{3+}/Yb^{3+} doping; tungstate

PP-46

A Visible Light-Promoted C-H Insertion Reaction of Diazoamides with 1,3-Diketones

Hariharan Selvaraj, *Muthusamy Sengodagounder**

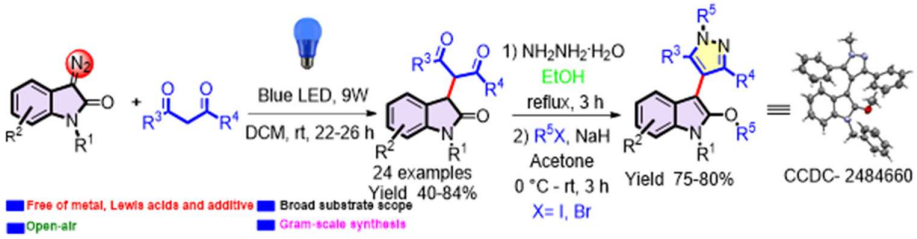
School of Chemistry, Bharathidasan University, Tiruchirappalli-620024, India.

E-mail: muthu@bdu.ac.in

Abstract: A visible light-promoted C-H insertion between diazoamides and 1,3-diketones leads to the corresponding 3-substituted-2-oxindoles in good yield. A subsequent reaction of the resulting product with hydrazine hydrate, followed by alkylation, provided biologically active 3-pyrazol-4-yl-indole derivatives in good to excellent yield, which can be easily scaled up to gram scale.

Oxindoles are important structural motifs commonly found in pharmaceuticals and natural products. The five-membered heterocycle pyrazole also represents a privileged structural unit that has attracted considerable attention due to its broad applications in medicinal, pharmaceutical, and agrochemical. Notably, the 3-pyrazol-4-yl-indoles framework exhibits significant cytotoxicity through tubulin inhibition and demonstrates potent anti-inflammatory activity as well as anti-HSV-1 properties.

Scheme



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PP-47

Sol-Gel synthesis of V_2AlC MAX Phase for multifunctional applications

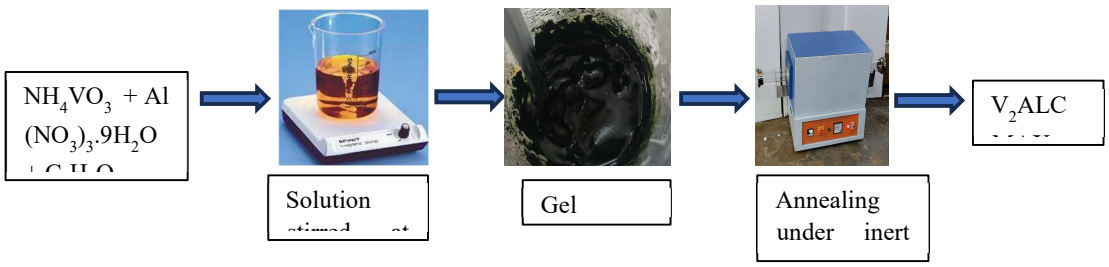
Aarthi.G and N.Sivanantham*

Division of Physics, School of Sciences, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Tiruchirappalli 621105, Tamilnadu, India

n.sivanantham@gmail.com

Abstract: Max Phases, a unique category of layered ternary carbides and nitrides, exhibit combined properties of metals and ceramics, making them a potential material for wide range of multifunctional applications. In the present work, V_2AlC Max phase was synthesized via Sol-gel method followed by heat treatment in an inert gas atmosphere [1]. The synthesized V_2AlC was characterized to analyse its structural, morphological, optical and functional properties. X-ray diffraction (XRD) analysis confirmed the formation of hexagonal V_2AlC MAX phase. Surface morphology analysis was done by Scanning electron microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDS) verified the elemental composition. Transmission Electron Microscope (TEM) further confirmed the crystalline nature of synthesized material. Identification of functional groups was done by Fourier Transform Infrared Spectroscopy (FTIR) and the optical behaviour was carried over by UV-Visible spectroscopy. The biomedical application of V_2AlC was explored by investigating the antibacterial activity against *E.coli* and *S.aureus* [2,3]. The photocatalytic performance was investigated through the degradation of Methylene blue (MB) and Rose Bengal (RB) dyes, and they exhibited efficient degradation performance. The obtained results highlight the potential of synthesized V_2AlC Max phase as a promising multifunctional material for antibacterial and photocatalytic applications.

Scheme:



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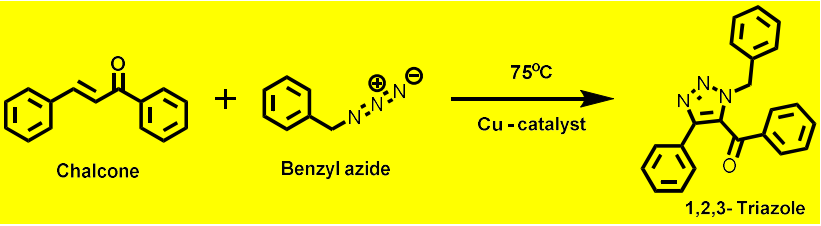
PP-48

Copper-Anchored Polyurethane Foams: Robust and Recyclable Heterogeneous Catalysts for Synthesis of Novel N-Heterocyclic Compounds

*Aishwarya S, Joydip Mondal and Dr. Akella Sivaramakrishna**
Department of Chemistry, School of Advanced Sciences, VIT, Vellore 632014, TN
asrkrishna@vit.ac.in

Abstract: Copper is one of the most abundant, significantly cost-effective, and more environmentally benign than noble metals. It exhibits a versatile redox chemistry associated with readily accessible multiple oxidation states (0, +1, +2, and +3), facilitating single-electron radical pathways as well as two-electron organometallic cycles. Also, copper displays high affinity for nitrogen donors and unsaturated alkenes and alkynes, which enables rapid C–N, C–C, and C–O bond constructions. [1] Recently, the focus has been mainly on designing copper complexes to enable efficient organic transformations, including A3-coupling, azide-alkyne cycloadditions/Click chemistry through multicomponent reactions (MCRs), intramolecular hydroamination, and C–H functionalization to construct fused heterocyclic rings. [2,3] Still, there is a strong demand for appropriate copper-based catalysts to minimize the usage of temperature and solvents, and to improve efficiency and selectivity in organic synthesis.

In view of this, the present work describes the synthesis of new copper-loaded functionalized polyurethane foams as efficient catalysts for the direct cyclization of precursors to form the corresponding N-heterocyclic compounds. These catalysts are reusable for more than 10 cycles. The factors such as stability aspects of the catalysts, density, and nature of ligand anchors, metal loading, solvent compatibility, steric and electronic properties of the reactants and other additives will be discussed. For example, the proposed catalysts offer a facile approach and are distinct from conventional azide–alkyne cycloadditions to obtain the targeted triazole frameworks. The copper-loaded polymer catalyst requires less time and exhibits excellent catalytic efficiency, operational simplicity, and reusability, with reduced copper leaching and cleaner product profiles.



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PP-49

Structural, Morphological and Luminescence study of Sm^{3+} doped $CaMgSi_2O_6$ Phosphor

Akshay Pimpalkar[1*], Nilesh Ugemuge[1*], Shruti Dhale[1,3*], Anil Muke[2],

[1]Department *of Physics, Anand Niketan College, Anandwan, Warora-442907, India*

[2]*Department of Physics, Avvaiyar Govt.College for Women, Karaikal-609602, India*

[3]*G H Raisoni College of Engineering, Nagpur, 440016, India*

***Corresponding Author:** Akshay Pimpalkar (akshaypimpalkar938@gmail.com),

Shruti Dhale (shrutidhale@gmail.com), Nilesh Ugemuge (nileshugemuge@gmail.com)

Abstract: In this study, $CaMgSi_2O_6:Sm^{3+}$ phosphor is synthesized using high-temperature solid state reaction (SSR) to investigate it's structural, morphological and photoluminescence properties. The XRD pattern confirmed the formation of $CaMgSi_2O_6$, exhibiting good agreement with the standard ICDD pattern, while it's crystal structure is also reported. SEM analysis revealed a porous, agglomerated and irregular surface morphology with interconnected microstructural features. EDS confirmed the presence of Ca, Mg, Si, and O, with elemental mapping demonstrating their homogeneous distribution throughout the $CaMgSi_2O_6$ matrix. Photoluminescence studies revealed characteristic Sm^{3+} excitation bands, with a prominent excitation at 400 nm ($^6H_{5/2} \rightarrow {}^4F_{7/2}$), while 400 nm excitation produced intense orange-red emission centered at 603 nm, corresponding to the $^4G_{5/2} \rightarrow {}^6H_{7/2}$ transition, with the emission intensity exhibiting a concentration-dependent behavior. The luminescence decay profile was analyzed to evaluate the excited-state lifetime of Sm^{3+}. These findings highlight the potential of $CaMgSi_2O_6:Sm^{3+}$ phosphor for applications in solid-state lighting, display technologies, and photonic devices.

Key Words: Photoluminescence; Sm^{3+} doping; silicate; phosphor

PP-50

Synthesis, Structural Characterization, DNA Interaction and Cytotoxicity Studies of Zinc (II) Azomethine Complexes

Anand Kumar Eswarasamy, Tharani Saravanan, Angappan Sheela*

Department of Chemistry, School of Advanced Sciences,
Vellore Institute of Technology, Vellore-632014, Tamil Nadu, India.
Email: asheela@vit.ac.in

Abstract: Azomethine based coordination compounds have been intensively studied for numerous commercial and medical purposes from long ago. These types of ligands and the metal center present in their complexes act synergistically in exerting their different biological functions. In the current study, we have synthesized and characterized a hitherto unreported ligands and the corresponding zinc complexes. The ligands is obtained from 4-nitro-o-phenylenediamine and 4-methyl-o-phenylenediamine react with 3,5-diiodo salicylaldehyde. The complexes are characterized by FTIR, NMR, UV, and HRMS spectroscopic techniques. The complexes possess potential oxygen and nitrogen binding sites for coordination with the metal center. The complexes are expected to possess binding interactions with the nucleic acids. The interaction with nucleic acid provides insight into the anticancer potential of the designed compounds. In this context, we have investigated the binding propensities of the complexes with DNA through UV absorption titration and fluorescence quenching assays.

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Keywords: Azomethine based ligands, Zn(II) complexes, DNA binding, cytotoxicity.

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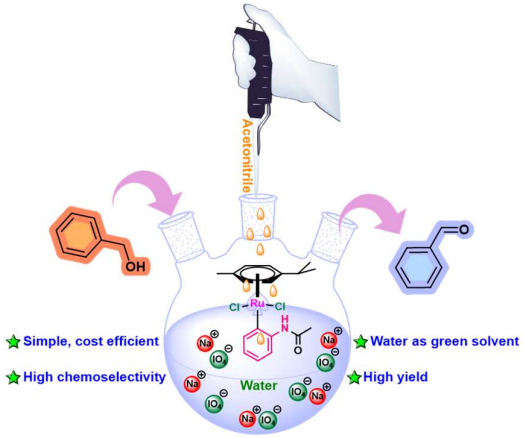
PP-51

Water-Compatible Phosphine-Free Ruthenium (II) Catalyst for the dehydrogenation of Benzyl Alcohol Derivatives in aqueous solution

Ashirbad Nayak [a], *Naveenkumar K*[a] and *Arup Sinha**[a]

[a] *Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, India. Email: ashirbad.nayak2024@vitstudent.ac.in, arup.sinha@vit.ac.in*

Abstract: The article addresses the development of a ruthenium arene complex (C1) utilising phosphine-free pyridine-based ligand. The complex was systematically characterised employing various spectroscopic techniques integrated with single-crystal X-ray crystallography, which validated its molecular structure. Additionally, a robust and efficient Ru (II)-catalyzed oxidation approach emerged for the selective transformation of alcohols into their respective carbonyl compounds under mild aqueous conditions. The catalytic system utilises sodium periodate ($NaIO_4$) as the ultimate oxidant in a water/acetonitrile solvent, offering an eco-friendly and straightforward methodology. The phosphine-free ruthenium catalyst demonstrated remarkable catalytic activity and chemo selectivity across an extensive variety of substrates, yielding the desired products in good to exceptional yields. The innovation shows numerous benefits, such as ecologically conscious reaction conditions, operational convenience, high efficiency, and superior selectivity, underlining the promise of phosphine-free Ru (II) complexes in sustainable catalytic oxidation processes.



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PP-52

Reduced graphene oxide-Polyoxometalate-Polypyrrole based high-performance electrode material for hybrid supercapacitors

Bency Jose[1], *Sib Sankar, Mal**[,1]
Materials and Catalysis lab, Department of Chemistry, National Institute of Technology, Karnataka-575025, India
bencyjose.247cy010@nitk.edu.in

Abstract: To address the low energy density limitation of EDLCs and pseudocapacitive materials and to achieve an optimal balance of electrochemical properties, an underexplored redox-active hybrid nanocomposite electrode material is fabricated for high-energy supercapacitors by incorporating polyoxometalates (POMs) and polypyrrole (PPy) into reduced graphene oxide (rGO). The synergistic interaction between the high surface area and electrical conductivity of reduced graphene oxide and the pseudocapacitive POM (Mo_4) and PPy contributes to the superior electrochemical performance of the nanocomposite. This study explores the ability of Mo_4 and PPy to enhance electrochemical performance by acting as interlayer spacers that increase interlayer spacing between rGO sheets, thereby preventing POM leaching and improving electrode surface wettability and specific surface area. In an aqueous 1 M H_2SO_4 electrolyte, the rGO-Mo_4-PPy supercapacitor cells demonstrate an energy density of 49.67 Wh kg-1, a power density of 1417.52 W kg-1, and a coulombic efficiency of 98.9% at a current density of 1 A g^{-1}. The hybrid supercapacitor cells exhibit relative diffusion and capacitive current contributions of 43% and 57%, respectively, at 2 mV s^{-1}. It reveals an exceptional capacitance retention of 82.5% after 5000 GCD cycles at a current density of 15 A g^{-1}.

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PP-53

Multifunctional Electrospun Bismuth substituted hydroxypatite/ ZnO/ PVA Nanocomposite for Bone Tissue Engineering Applications

*Bhagyashree V and S. Sumathi**

Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu, India, ***Email:*** *bhagyashree.v@vit.ac.in*

Abstract: Bone tissue engineering demands multifunctional scaffolds that can simultaneously promote bone regeneration, prevent bacterial infection, and provide sufficient mechanical support. In this work, a novel electrospun nanofibrous composite comprising bismuth-substituted hydroxyapatite (Bi-HAP), zinc oxide (ZnO), and polyvinyl alcohol (PVA) was developed. Bi-HAP serves as a bioactive ceramic that mimics the mineral phase of natural bone. ZnO was added to impart antibacterial activity. PVA was employed as a biodegradable polymeric matrix to improve flexibility and fibre formation, enabling the fabrication of interconnected nanofibrous scaffolds by electrospinning. The fabricated electrospun composites were systematically characterized using P-XRD, FT-IR, and SEM to elucidate their structural, chemical, and morphological features. Their functional performance was further assessed through porosity, tensile strength, antibacterial activity, in-vitro hemocompatibility, and in-vitro cytocompatibility studies. The synergistic integration of Bi-HAP, ZnO, and PVA is expected to create a multifunctional composite with enhanced bioactivity, antibacterial activity, mechanical strength, and cell viability.

Keywords: Bismuth-substituted hydroxyapatite; Zinc oxide; Polyvinyl alcohol; Electrospinning; Nanofibrous composite; Bone tissue engineering.

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PP-54

Morphology-Controlled $CoFe_2O_4$ through Surfactant-Mediated Synthesis for Enhanced Electrochemical Performance in Asymmetric Supercapacitors

Divya T, Sivakami A
Department of Physics, Sri Eshwar College of Engineering, Kinathukadavu, Coimbatore – 641 202, Tamil Nadu, India.
Presenting Author E-mail: divya.t@sece.ac.in
Corresponding Author E-mail: sivakami.a@sece.ac.in

Abstract: Developing electrode materials with improved charge-storage capability is essential for advancing supercapacitor technology. In this study, $CoFe_2O_4$ electrodes were synthesized via a simple wet-chemical route using three surfactants cetyltrimethylammonium bromide (CTAB), polyethylene glycol (PEG) and sodium dodecylbenzene sulfonate (SDBS) as structure-directing agents, each yielding distinct surface morphologies. FTIR and XRD analyses confirmed the characteristic metal-oxygen (Fe–O and Co–O) vibrational bands and verified formation of a cubic spinel $CoFe_2O_4$. BET measurements revealed variations in surface area and pore features depending on surfactants used, while FE-SEM analysis evidenced the corresponding morphological differences. Among the electrodes, CTAB-assisted $CoFe_2O_4$ displayed an interconnected nonspherical morphology and delivered highest specific capacitance of 570 F g^{-1} at 2 A g^{-1}, retaining about 83 % of its initial capacitance after 3000 charge-discharge cycles. An asymmetric device was assembled using $CoFe_2O_4$ and activated carbon as the positive and negative electrodes, respectively, delivered a specific capacitance of 94 F g^{-1} at 2 A g^{-1} with an energy density of 22 Wh kg^{-1} at a power density of 2640 W k g^{-1}. These results confirm that surfactant-assisted morphological tuning of $CoFe_2O_4$ offers an effective strategy for enhancing charge-storage performance, marking a promising route for future supercapacitor electrode development.

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PP-55

$NdCoP_2O_7$ Microrods Integrated with an Interconnected Carbon Nanofiber (CNF) Network for Asymmetric Supercapacitor

*Boopathi Bommu, Suresh Rajan**

Department of Physics, Sri Eshwar College of Engineering (Autonomous), Coimbatore, 641202, Tamil Nadu, India.

Presenting author E-mail: boopathir382@gmail.com

**Corresponding author E-mail: suresh.r@sece.ac.in*

Abstract: Designing high-performance electrode materials continues to play a pivotal role in hybrid supercapacitor devices. In this study, we synthesized a composite of $NdCoP_2O_7$ and carbon nanofibers (CNF) using a single-step hydrothermal process combined with probe sonication. A range of structural and spectroscopic techniques confirmed both the successful crystallization of $NdCoP_2O_7$ and its effective integration with the CNF matrix. The phase purity of $NdCoP_2O_7$ was established through XRD analysis, whereas FTIR and Raman spectra revealed distinct vibrational signatures corresponding to Nd-O, Co-O, and P-O-P bonds, alongside the D and G bands characteristic of the carbon framework. XPS analysis provided further insight into the oxidation states of Nd and Co, confirming their contribution as active redox sites within the composite. Morphological analysis via FE-SEM and HR-TEM revealed that the one-dimensional $NdCoP_2O_7$ microrods were well dispersed across the CNF network, forming an interconnected and highly conductive hybrid architecture. This structural synergy translated into strong electrochemical performance, with the composite attaining a specific capacitance of 850 F g^{-1} at a current density of 0.5 A g^{-1}. When integrated into an R2032-type asymmetric coin cell, the device delivered a capacitance of 190 F g^{-1} at 0.5 A g^{-1} and an energy density of 85 Wh kg^{-1} at a power density of 690 W kg^{-1}. Notably, the cell retained 94% of its initial capacitance and maintained a coulombic efficiency of 99% over 10000 charge–discharge cycles, underscoring its excellent cycling stability. To highlight its real-world applicability, three such cells connected in series were successfully used to power red, orange, yellow, and green LEDs.

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PP-56

Interfacially Engineered Silver-Ruthenium Nanoparticle-Anchored Borophene for Enhanced Antibacterial Activity and Breast Cancer Cell Inhibition

Krithikapriya Chinniah [a], *Sundrarajan Mahalingam* [a,*]

[a]*Advanced Green Chemistry Lab, Department of Industrial Chemistry, School of Chemical Sciences, Alagappa University, Karaikudi - 630 003, Tamil Nadu, India.*

E-mail: sundrarajanm@alagappauniversity.ac.in; drmsgreenchemistrylab@gmail.com

***Corresponding author:** M. Sundrarajan*

Abstract: Despite borophene's (Bp) exceptional physicochemical qualities, rapid oxidation, structural instability, limited dispersibility, and inadequate biological activity hinder its effective biomedical applications. Similarly, monometallic silver (Ag) and ruthenium (Ru) nanoparticles (NPs) frequently exhibit poor multifunctionality, decreased stability, and aggregation, which limit their long-term performance. Ag-Ru NPs anchored Bp nanosheets (Ag-Ru/Bp) nanocomposite (NC) was created utilizing a green ultrasonication-aided in situ synthesis technique to overcome these restrictions. *Nyctanthes arbor-tristis* (*NAT*) floral extract was used as a natural reducing, capping, and stabilizing agent. In situ growth of Ag-Ru NPs on the Bp surface successfully inhibited NPs aggregation, increased interfacial coupling, and structural stability, resulting in a uniformly distributed bio capped NC. Strong interactions among *NAT* phytochemicals, Ag-Ru nanoparticles (Ag-Ru NPs), and borophene nanosheets (Bp NSs) were evidenced by characteristic spectral shifts. FTIR analysis confirmed the involvement of *NAT* phytochemicals in the green reduction, stabilization, and surface functionalization of the Ag-Ru NPs. Furthermore, SEM, TEM, HRTEM, SAED, EDX, and elemental mapping revealed the homogeneous distribution of highly crystalline Ag-Ru NPs with an average particle size of 12.39 nm on the Bp NSs, while XRD analysis further confirmed the crystalline nature of the Ag-Ru/Bp nanocomposite

Keywords: Borophene nanosheets; *Nyctanthes arbor-tristis* extract; Silver/Ruthenium nanoparticles; Biointerface interactions; Anticancer and Antibacterial activity.

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PP-57

Facile Synthesis of $NiVO_4/SnO_2$ Heterostructure Nanocomposite as a High-Performance Electrode Material for Supercapacitor Applications

*Aswini Ravi, Ganesh Kumar V**
Centre for Ocean Research, Sathyabama Institute of Science and Technology, Chennai-600119, India
**ganeshkumar@sathyabama.ac.in*

Abstract: The increasing demand for high-performance energy storage devices has created a need for electrode materials with high capacitance, rapid charge transport, and good cycling stability. In this work, a $NiVO_4/SnO_2$ heterostructure nanocomposite was prepared through a simple and economical synthesis route for supercapacitor applications. The integration of SnO_2 with $NiVO_4$ improves the structural stability of the electrode while increasing the number of electrochemically active sites. The close contact between the two metal oxides promotes efficient electron transfer and shortens the ion diffusion pathway, leading to improved electrochemical kinetics. Owing to the synergistic interaction between $NiVO_4$ and SnO_2, the composite exhibits enhanced charge storage behaviour, higher specific capacitance, improved rate performance, and better cycling stability than the individual components. The heterostructure also helps maintain the integrity of the electrode during repeated charge–discharge cycles by reducing structural degradation and facilitating reversible redox reactions. As a result, the composite retains its electrochemical performance over extended cycling. The overall results demonstrate that the $NiVO_4/SnO_2$ heterostructure is a promising electrode material for advanced supercapacitors and offers a practical strategy for the development of efficient and durable electrochemical energy storage devices.

Keywords: $NiVO_4$; SnO_2; Heterostructure nanocomposite; Supercapacitor; Electrochemical energy storage; Cycling stability

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PP-58

Interface-Engineered $Co_2V_2O_7$@rGO Nanocomposite for Enhanced Bifunctional Electrocatalysis toward Overall Water Splitting

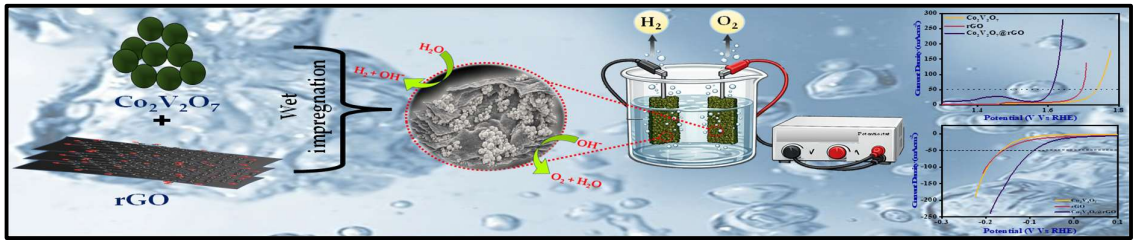
*Harini Bhagyaraj, Nithesh Kumar Krishnan, Stalin Thambusamy**

Department of Industrial Chemistry, Alagappa University, Karaikudi - 630 003, Tamil Nadu, India.

Presenting author E-mail: harinibhagyaraj01@gmail.com

**Corresponding author E-mail: stalin.t@alagappauniversity.ac.in*

Abstract: The development of efficient, low-cost, and durable electrocatalysts is crucial for sustainable hydrogen production through alkaline water electrolysis. Although cobalt vanadates show promising catalytic properties, their performance in hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) is significantly hampered by the poor intrinsic electrical conductivity and limited electrochemically active surface area of pristine $Co_2V_2O_7$. In this study, we synthesized a reduced graphene oxide (rGO)-supported $Co_2V_2O_7$ nanocomposite to enhance conductivity and provide abundant active sites. We investigate its bifunctional electrocatalytic performance for HER, OER, and overall water splitting using both hydrothermal and ultrasonication methods. X-ray diffraction (XRD) results indicate the presence of highly crystalline $Co_2V_2O_7$, along with a broad diffraction peak related to amorphous rGO, suggesting the formation of a hybrid composite with both crystalline and amorphous phases, which aligns with the selected area electron diffraction (SAED) pattern. Additionally, shifts in Raman bands and corresponding changes in binding energy observed in X-ray photoelectron spectroscopy (XPS) indicate a strong electronic interaction between $Co_2V_2O_7$and rGO. Scanning electron microscopy-energy dispersive X-ray spectroscopy (SEM-EDX) and high-resolution transmission electron microscopy (HRTEM) reveal that the quasi-spherical $Co_2V_2O_7$ nanoparticles are uniformly distributed on the layered sheet-like structure of rGO. The $Co_2V_2O_7$@rGO nanocomposite demonstrates excellent bifunctional electrocatalytic activity, requiring an overpotential of 83 mV at a current density of 50 mA cm^{-2}, with a Tafel slope of 103 mV/decade. It also exhibits robust OER performance of 370 mV at 50 mA cm^{-2}, with a Tafel slope of 55 mV/decade. An assembled two-electrode electrolyzer achieved a cell voltage of 1.68 V at 10 mA cm^{-2}, underscoring its superior bifunctional performance. These findings position $Co_2V_2O_7$@rGO as a promising, earth-abundant, and durable bifunctional electrocatalyst, offering significant potential for future renewable hydrogen production technologies.



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PP-59

Harnessing UV Light to Create Oxygen Vacancy-Enriched Black BiOCl for Enhanced Visible-Light Photocatalytic Degradation of Rhodamine-B.

Johan Oommen Cherian [1], *Steffy Mariyam Varghese* [1], *Akshay M Achari* [2], *Swati G* [2]*
[1] *Department of Chemistry, SAS, Vellore Institute of Technology, Vellore, 632014*
[2] *Centre for Nanotechnology Research (CNR), Vellore Institute of Technology, Vellore, 632014*
**swati.g@vit.ac.in*

Abstract: Bismuth oxychloride (BiOCl) is a potent semiconductor photocatalyst, but its wide band gap limits its efficacy under visible light[1]. This study demonstrates a novel approach using UV-induced defect engineering to create controlled oxygen vacancies, thereby enhancing BiOCl's visible-light activity. BiOCl was synthesized via a one-pot coprecipitation method. As obtained, pristine BiOCl was irradiated with UV-C (254 nm) light for various durations to examine the effects on its structural, optical, and photocatalytic properties. X-ray diffraction (XRD) confirmed that UV treatment maintained BiOCl's crystal structure, with modifications occurring at the surface. UV–Vis diffuse reflectance spectra showed increased absorption in the visible range, and photoluminescence (PL) studies revealed reduced charge recombination for the irradiated sample. Samples irradiated for 10 hours showed promising photocatalytic degradation of Rhodamine B. Further increasing the duration of irradiation reduced the performance due to the introduction of excessive oxygen vacancies that introduce recombination centres[2,3]. This research offers a straightforward and effective strategy for enhancing BiOCl through self-induced defect engineering, providing valuable insights into its photocatalytic mechanisms and promoting its application in environmental remediation.

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PP-60

SO_3H@Carbon Powder Derived from Waste Cassava Peel: An Efficient, Recyclable Green Catalyst for the Ultrasound-Assisted Synthesis of (phenylamino)-1,4,5,6,7,8-hexahydroquinoline-3-carbonitrile Derivatives

Ponmalai Kavina[1] and Appaswami Lalitha[1*]

[1]*Department of Chemistry, Periyar University, Salem-636011, Tamil Nadu, India.*

**Corresponding author e-mail: lalitha2531@yahoo.co.in, Tel: +91-427-234-5271; Fax: +91-427-234-5124*

Abstract: The development of sustainable and environmentally benign catalytic systems from biomass waste has emerged as an important strategy in green organic synthesis. In this work, a recyclable sulfonated activated carbon catalyst (CPC–SO_3H) was successfully prepared from waste cassava peel and employed for the ultrasound-assisted one-pot three-component synthesis of (phenylamino)-1,4,5,6,7,8-hexahydroquinoline-3-carbonitrile derivatives in a green solvent. The reaction conditions were systematically optimized by varying the reaction temperature, catalyst loading, reaction time and ultrasound irradiation to obtain the desired products in excellent yields within a short reaction time. The synthesized catalyst was comprehensively characterized by FT-IR, XRD, SEM, EDX, BET, XPS and TGA–DTA analyses, confirming the successful incorporation of sulfonic acid functionalities and its good thermal stability. A series of (phenylamino)-1,4,5,6,7,8-hexahydroquinoline-3-carbonitrile derivatives was synthesized using various substituted aromatic aldehydes and characterized by FT-IR, ^1H NMR and ^{13}C NMR analysis of a representative compound. The catalyst exhibited excellent catalytic efficiency, operational simplicity, easy recovery, and reusability, demonstrating its potential as a sustainable heterogeneous solid-acid catalyst. This study highlights the value of waste cassava peel as a renewable precursor for the preparation of efficient biomass-derived catalysts and provides an environmentally friendly approach for the synthesis of biologically important (phenylamino)-1,4,5,6,7,8-hexahydroquinoline-3-carbonitrile derivatives.

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PP-61

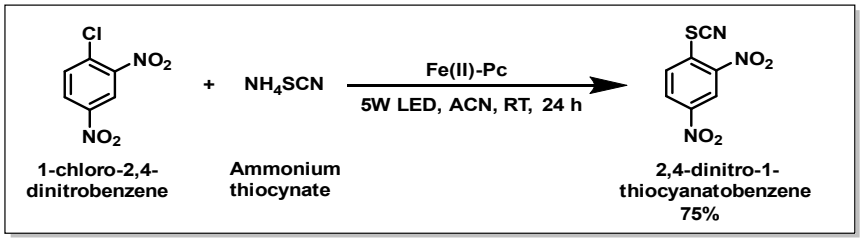
Visible-Light-Induced Thiocyanation of Aryl Halide Using a Recyclable Fe(II)-Porphyrin Heterogeneous Photocatalyst

Kiran Vilas Butle, *Anurag Vinayak Pujari* and *Pundlik Rambhau Bhagat**
[a] Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, India.

*Corresponding author: drprbhagat111@gmail.com, pundlik.rb@vit.ac.in (Pundlik Rambhau Bhagat)

Abstract: Developing sustainable methods for C–S bond formation remains an important objective in organic synthesis because aryl thiocyanates are versatile intermediates for pharmaceuticals, agrochemicals, and functional materials. In this work, a recyclable Fe(II)-porphyrin heterogeneous photocatalyst (Fe(II)-Pc) was achieved by coordinating ferrous sulfate with a sulfonic acid-functionalized porphyrin containing benzo-triazolium moiety. The photocatalytic performance of Fe(II)-Pc was evaluated for the thiocyanation of activated aryl halides under visible-light irradiation using ammonium thiocyanate (NH_4SCN) as the thiocyanate source. Under optimized conditions, 1-chloro-2,4-dinitrobenzene was converted into 2,4-dinitro-1-thiocyanatobenzene in acetonitrile under a 5 W LED at room temperature in 24 h. The catalyst promoted efficient C–S bond formation under mild reaction conditions without the use of harsh oxidants or elevated temperatures. These findings demonstrate that Fe(II)-Pc is a promising recyclable heterogeneous photocatalyst for visible-light-driven thiocyanation, offering a simple and environmentally friendly approach for the synthesis of aryl thiocyanates.

Scheme:



Scheme 1: Synthesis of 2,4-dinitro-1-thiocyanatobenzene

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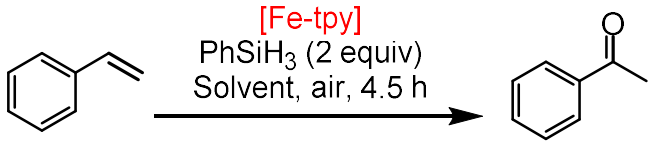
PP-62

Redefining Wacker Oxidation Chemistry: Sustainable Iron Catalysis at Room Temperature

*Kishore Raghu, Rakesh R Panicker, Akella Sivaramakrishna**
Department of Chemistry, School of Advanced Sciences, VIT, Vellore 632014, TN
asrkrishna@vit.ac.in

Abstract: The Wacker oxidation—traditionally the palladium-catalyzed, copper-mediated conversion of terminal alkenes into methyl ketones—has undergone a major paradigm shift. Recent developments focus on overriding classical Markovnikov regioselectivity, expanding substrate scope beyond terminal alkenes, eliminating expensive or toxic palladium/copper co-catalyst systems, and adopting greener aerobic oxidation conditions. The advances include anti-Markovnikov regioselectivity for the development of ligand-controlled and directing-group-assisted palladium systems that selectively yield aldehydes over methyl ketones from terminal alkenes. Further, extension of Wacker-type oxidations to internal, 1,1-disubstituted, trisubstituted, and tetrasubstituted alkenes is a challenging task. Notably, there is a strong demand for a sustainable and palladium-free catalysis to replace scarce, toxic palladium complexes with earth-abundant first-row transition metals (*e.g.,* iron, cobalt, nickel) and to exchange corrosive copper salts with an alternative. In this regard, a series of novel functionalized terpyridine ligands was synthesized *via* an efficient synthetic protocol and subsequently coordinated with Fe (III) ions to afford structurally well-defined iron–terpyridine coordination complexes for catalytic investigations. The synthesized ligands and their corresponding iron complexes were characterized using spectroscopic and analytical techniques. The catalytic performance of the complexes was evaluated using the Wacker oxidation reaction under optimized conditions. The results showed that systematic functionalization of the terpyridine framework modulates the electronic environment of the iron center, leading to enhanced catalytic activity with high selectivity. These findings demonstrate the crucial role of ligand design in improving catalyst performance while utilizing earth-abundant iron as an environmentally friendly alternative to noble metals. This study provides valuable insights into the development of efficient terpyridine-based catalytic systems for sustainable homogeneous catalysis and advanced coordination chemistry.

Figure/Scheme:



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PP-63

Metal oxide-MOF Composite for Rapid Hydrogen Sensing under Oxygen-deprived Environments at Ambient Conditions

*Ganesh Korada,[a] Krishnaveni Valle,[a] A Sree Rama Murthy,[b] V. Jayaraman,[b] Kiran Vankayala,[c] Suresh Babu Kalidindi[a]**

a. Department of Chemistry, Central Tribal University of Andhra Pradesh (CTUAP), Kondakarakam, Cantonment Area, Vizianagaram, Andhra Pradesh, 535 003, India
b. Material Chemistry Division, Materials Chemistry and Metal Fuel Cycle Group, Indira Gandhi Centre for Atomic Research, Kalpakkam 603 102, India
c. Functional Materials for Electrochemistry and Solar energy (FunMatES) Group, Energy and Environmental Chemistry Lab, Department of Chemistry, Birla Institute of Technology & Science, Pilani, K. K. Birla Goa campus, Goa, 403 726, India
Email: ksureshu@gmail.com/suresh.babu@ctuap.ac.in

Abstract: Hydrogen has gained significant global interest as a clean energy carrier because its combustion byproduct is environmentally benign water. It has great potential to replace fossil fuels. However, its high flammability range (4-75%) demands rapid leak detection for safe operation and to prevent explosions. Chemiresistive sensors have gained more attention because of their simple device fabrication, low cost, and fast response. Hydrogen sensing under oxygen-deprived environments is becoming a more interesting area, and it is essential to maintain safe operations such as hydrogen fuel cell systems and fast nuclear reactors. However, most of the hydrogen sensors are designed to operate in oxygen-containing environments, while hydrogen detection under inert or oxygen-deprived environments is rarely reported. Therefore, the development of rapid hydrogen sensors capable of operating in inert atmospheres is crucial for various applications.[1] Among various sensing materials studied, n-type SnO_2 has emerged as one that clearly stands out as the most prominent candidate, owing to its attractive features such as low cost, excellent stability, and simple fabrication, despite having drawbacks such as high operational temperature and the requirement for an oxygen atmosphere. In this work, we designed a novel heterostructure sensor by integrating n-type SnO_2 thin films with p-type conductive $Cu_3(HHTP)_2$ MOF for effective hydrogen sensing under an argon atmosphere.[2] Electron-beam-grown pristine SnO_2 films were insensitive to hydrogen at RT. However, deposition of $Cu_3(HHTP)_2$ over SnO_2 generated p-n heterojunction interfaces that enabled sensing behavior even in the absence of oxygen. At RT, the exfoliated $Cu_3(HHTP)_2$ exhibited a response (R%) of 1.5 toward 0.1% H_2 with fast response and recovery times of 1.1 s each, the sensors showed a positive sigmoidal response at room temperature. Pristine SnO_2 remained inactive. The SnO_2film@$Cu_3(HHTP)_2$ composite demonstrated significantly enhanced sensing performance with an R% of 7.5, response time of 6 s, and recovery time of 8.2 s under argon, accompanied by a negative sigmoidal response indicative of dominant n-type behavior. Detailed structural, morphological, surface characterization, and gas sensing studies of all materials will be presented in the poster.

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PP-64

Synthesis of a Nitrogen-Rich Hydrazone-Based Metal-Organic Framework for Fluorescent Carbon Monoxide Sensing

*Moorthy Rishi Sanjay & Subramanian Karpagam**

Department of Chemistry, School of Advanced Sciences, Vellore Institute Of Technology, Vellore -14 ,Tamil Nadu, India, skarpagam80@yahoo.com, skarpagam@vit.ac.in

Abstract: A nitrogen-rich fluorescent ligand was synthesised through a concise multistep strategy involving N-alkylation, formylation and subsequent hydrazone formation. Diphenylamine was Nalkylated, followed by formylation to afford N-butyl-4-formyldiphenylamine. Condensation with hydrazine-hydrate and subsequent functionalisation with 2-hydroxynaphthaldehyde afforded a πconjugated hydrazone ligand containing multiple nitrogen and oxygen donor sites. The ligand was further employed in the construction of a copper-based metal–organic framework in the presence of Cu_2O and benzene-1,3,5-tricarboxylic acid, yielding crystalline MOF materials. The photophysical properties of the resulting material were investigated towards carbon monoxide sensing. Upon exposure to CO, a pronounced fluorescence quenching response was observed, demonstrating the potential of this fluorescent MOF platform for CO detection. This study highlights the utility of integrating π-conjugated hydrazone ligands with metal–organic frameworks to develop responsive fluorescent materials for gaseous analyte sensing.

Keywords: Metal–organic frameworks, Carbon monoxide sensing, Hydrazone ligand, Fluorescence quenching, Copper-MOF.

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PP-65

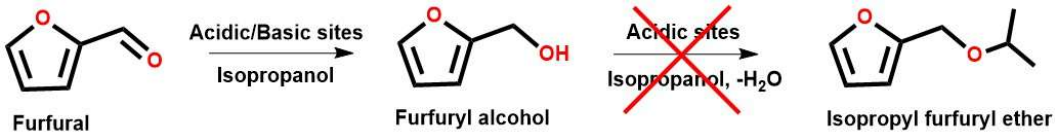
Selective conversion of furfural to furfuryl alcohol using yttrium aluminates

*Monish Ramakrishnan, Neha Choudhary, Mohammed Abbas Akhtar Hasnain, and Cheralathan Kanakkampalayam Krishnan**

Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology (VIT), Vellore - 632 014, India

**Corresponding author email ID: cheralathan.k@vit.ac.in (Cheralathan K K)*

Abstract: Yttrium aluminate catalysts with varied Y/Al ratios were synthesised by co-precipitation and evaluated for the catalytic transfer hydrogenation of furfural to furfuryl alcohol using isopropanol (IPA) as the hydrogen donor. Among the catalysts, YA-3:1 showed the highest activity, achieving 77.2% furfural conversion and 73% furfuryl alcohol yield with 95% selectivity. Characterization and active site-poisoning studies revealed that the enhanced performance originated from an optimized balance of surface acid-base sites, which promoted selective furfuryl alcohol formation while suppressing side reactions. Catalyst deactivation upon recycling was attributed to carbonate accumulation on basic sites and was completely reversed by regeneration at 600 °C. These results demonstrate the potential of yttrium aluminate catalysts for selective biomass-derived furfural valorization.



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PP-66

Design, Synthesis and Photophysical Studies of some Mixed-Ligand Transition Metal Complexes: Experimental and DFT Insight

Naman Arora, *Jyoti Kandhal, Jitander Kumar Kapoor and Minati Baral*[*]

Department of Chemistry, National Institute of Technology, Kurukshetra, Haryana-136119, India
email: minatibnitkkr@gmail.com

Abstract: A novel series of mixed-ligand metal complexes of the type $ML_1L_2L_3$, where M = Zn^{+2}, Cu^{+2}, Ni^{+2}, Co^{+2} and Fe^{+2}; L_1= Salicaldehyde thiosemicarbazone (Sal-TSC), L_2=Triphenylphosphine oxide (TPPO), and L_3= 8-hydroxyquinoline (8HQ). The complexes were characterized using different analytical techniques such as FTIR, UV-Vis, ESI-MS, NMR, and TGA. The results confirmed the chemical formulation of mixed transition metal complexes(1). The spectral and computational studies revealed all the complexes adopting distorted octahedral geometries, coordinating through nitrogen, sulfur, and oxygen donor atoms. With distorted octahedral geometries. Photophysical studies showed an enhancement (1.42-fold) in the fluorescence intensity of the ligand-centric emission in the case of the Zinc complex only, whereas other metal complexes did not show any significant changes in the emission spectra. Additionally, the zinc complex exhibited anion selectivity, with a significant fluorescence enhancement in the presence of fluoride ions, which can be rationalized through CHEF and PET mechanisms (2). Density functional theory (DFT) studies conducted using the GGA-BLYP-D3 functional with a TZP basis set explored the structural and bonding behavior of the metal complexes. The DFT calculations supported the experimental findings, such as FTIR and electronic spectra . Advanced bonding analyses such as natural bond orbital (NBO) and energy decomposition analysis with extended transition state-natural orbitals for chemical valence (EDA-ETS-NOCV) provided insights into bonding, donor-acceptor interactions, and covalency in these metal complexes

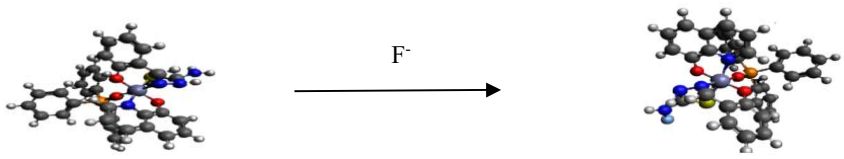

Figure 1. An illustration diagram of the interaction of the Zn(Sal-TSC)(8HQ)(TPPO) complex with F^- ions.

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PP-67

Supramolecular Engineering of γ-Cyclodextrin Encapsulated Rhodamine Derivative Modified Histidine Porous Carbon for Solid-State and $LiPF_6$ Symmetric Supercapacitors

*Nithesh Kumar Krishnan, Stalin Thambusamy**
Department of Industrial Chemistry, Alagappa University, Karaikudi - 630 003, Tamil Nadu, India.
Presenting author E-mail: nitheshkumar@alagappauniversity.ac.in
**Corresponding author E-mail: stalin.t@alagappauniversity.ac.in*

Abstract: In this work, a novel strategy is employed to prepare the mesoporous carbon materials using supramolecular chemistry. The hazardous rhodamine dye (E)-3',6'-bis (diethylamino)-2-((2-nitrobenzylidene) amino) spiro [isoindoline-1,9'-xanthen] -3-one (N-RB) was synthesized by a two-step process and confirmed, and it was encapsulated into the γ-cyclodextrin (γ-CD) cavity, as confirmed by theoretical and spectroscopic techniques. The γ-CD/N-RB selectively detects L-Histidine (L-His), as confirmed by the UV-Visible and fluorescence spectra, with detection limits of 6.34×10^{-7} and 4.48×10^{-7} M, respectively, without any interference with other amino acids. The γ-CD/N-RB/L-His was hydrothermally treated, yielding Cγ-CD/N-RB/L-His porous carbon. The electrochemical analysis of Cγ-CD/N-RB/L-His demonstrates a specific capacitance of 911 F/g at a current density of 1 A/g in a 1 M KOH electrolyte, with a capacitance retention of 93% over 10,000 cycles. The symmetric supercapacitor analysis was conducted for all the carbon materials. The configuration Cγ-CD/N-RB/L-His//PVA-KOH//Cγ-CD/N-RB/L-His achieved an impressive energy density of 57 Wh/kg and a power density of 1200 W/kg, with a capacitance retention of 91% over 10,000 cycles. Additionally, real-time LED illumination studies were performed. Using a non-aqueous LiPF6 electrolyte, the device attained a potential window of 2.8 V, delivering an energy density of 33.4 Wh/kg at a power density of 1400 W/kg, with a capacitance retention of 98% over 2,000 cycles.

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PP-68

Immobilization of Mo(VI) in $La(OH)_3$ Lattice for Radioactive Molybdenum Confinement

Ponnarasan Subramani [a], *Srinithi Karthikeyan* [a], *Shumugtha Shanmugam* [a], *and Buvaneswari Gopal* [a]*

[a] *Department of Chemistry, Vellore Institute of Technology, Vellore, Tamil Nadu, India.*
**E-mail: gbhuvaneswari@vit.ac.in*

Abstract: Nuclear energy is an essential source of global electricity, while the safe disposal of radioactive waste remains critical. There are 438 Operational nuclear reactors used worldwide; The total electricity generation was 14% of the global supply and 3% of our own country's supply. The main fuels are uranium, plutonium, and thorium. These fuels undergo nuclear fission reaction, releasing massive amounts of heat energy and producing a large number of fission products (FPs), those (FPs) radioactive isotopes are typically radioactive. Molybdenum is one of the main fission Products of the Uranium Reduction Extraction [PUREX] process for highly enriched uranium and low-enriched uranium. These Molybdenum radioisotopes are present in high-level waste, intermediate-level waste, low level waste. The Long-term storage of Mo radioactive waste leads to Environmental Contamination, Radiation burns, Occupational hazards, high risk of Cancer, and other long-term health issues. Molybdenum radioisotopes present in Molybdate $(MoO_4)^{2-}$ form in uranyl nitrate nuclear waste solution. Hence, removing Mo(VI) is consequential due to concerns regarding environmental and human health. Multiple techniques are utilized to remove Mo(VI) oxyanions. The current study presents an integrated approach for the removal of Mo(VI) in aqueous media and then immobilization using $La(OH)_3$. The Immobilization process effectively restricted the release of Mo(VI) under real-world environmental conditions. This functional material offers a promising route for safe immobilization of Mo(VI) from nuclear waste, aligning with long-term strategies for radioactive waste minimization and sustainable environmental remediation.

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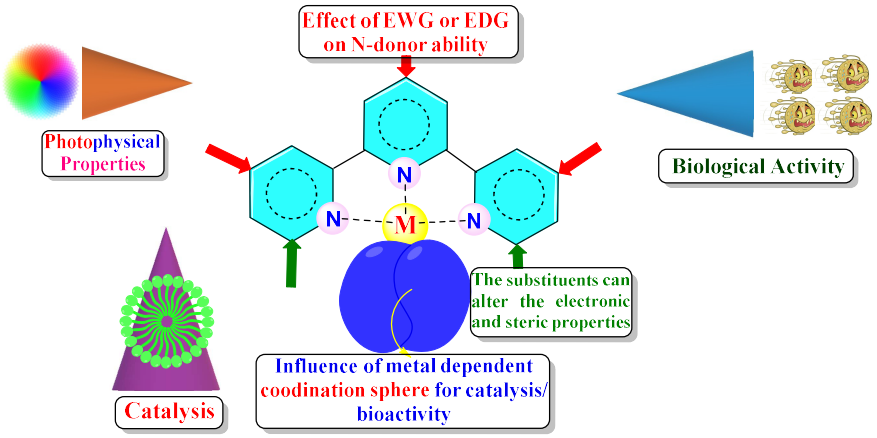
PP-69

Molecular Tuning: Functionalized Terpyridine Frameworks for Advanced Catalytic and Sensing Platform

Praveena B*, Rakesh R. Panicker, and Akella Sivaramakrishna
Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu

Abstract: Terpyridines (tpy) are versatile N3-chelating ligands capable of strong, tight coordination with diverse metal cations. Their electron-deficient pyridine rings render them weak σ-donors but strong π-acceptors, while their flexible redox behaviour has enabled numerous catalytic applications in organic transformations. Notably, tpys also support the construction of attractive supramolecular coordination polymers. A thorough literature survey on tpy-based Group 8–10 metal complexes reveals their broad contributions to catalysis and biological activity. New terpyridine ligands and their corresponding metal complexes were synthesized, and their structures were confirmed through a range of analytical and spectroscopic techniques. In view of this, selected tpy ligands and the corresponding Ni(II) complexes were prepared and their usage as catalysts in ethylene oligomerization reactions was studied. Notably, the nature of ligands as well as temperature strongly influence the organic product distribution, *i.e.* elevated temperatures facilitate 1-hexene (C6) as a significant product. Among all the complexes, the Ni(II)-tpy substituted with 5-chloro-thiophenyl group at 4′ position showed high selectivity for 1-hexene (C6, 80%) at room temperature and 1-octene (C8, 91%) at elevated temperatures. Though both mechanistic pathways were proved to be feasible, the present study is also intended to identify and analyze the key intermediate species of the reactions. Also, the modified terpyridine ligand was useful as a fluorescence-based sensing platform for selective metal ion detection.

Figure/Scheme:



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PP-70

Tailored *α*-Aminophosphonates: Unlocking Superior Coordination, Photophysical, and Biological Properties

*Preethi M, A.S. Vijai Anand, Rajagopal Desikan, and Akella Sivaramakrishna**
Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology (VIT), Vellore 632 014, Tamil Nadu, India

Phosphine oxides are very well-known to exhibit remarkable coordination behaviour, photophysical, catalytic and biological properties including rich structural architectures. Among these interesting organophosphorus family, α-aminophosphonates are unique class of compounds due to the presence of additional N atom(s) responsible for their improved biological and catalytic activities. Since, a subtle change in the electronic and steric properties of remote substituents leads to the hitherto unknown properties, there is a strong demand for the synthesis of new aminophosphonates in search of promising candidates as ligands in coordination chemistry, probes for chemosensors, catalysts for organic transformations including for biological applications. In this regard, the present work is focused on the synthesis of various α-aminophosphonates by a streamlined three-component Kabachnik–Fields synthetic approach under mild conditions driven by a Lewis acid in ethanol at ambient temperature. The products were isolated in high yields (87–95%), accommodating a wide range of ring-substituted substrates and the structural characterization was achieved through various spectroscopic and analytical techniques including single-crystal X-ray diffraction analysis. Cyclic voltammetry revealed that the ferrocene moiety contributes a distinct redox behaviour, modulated by molecular substitutions. A comparison was made among various phosphine oxides and α-aminophosphonates in terms of coordination strength with selected *f*-metals. The bioactivity studies of selected α-aminophosphonates revealed that they exhibit anti-cancer activity.

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PP-71

Hydrothermally Synthesized $CoMoO_4/TiO_2$ Heterostructure as an Efficient Electrocatalyst for Hydrogen Evolution Reaction

P. Ragul[1], *P. Velusamy*[1*]

[1]*Department of Physics, Thiagarajar College of Engineering, Madurai-625015, Tamil Nadu, India.*

Correspondence E-mail: velusamy.phy@gmail.com

Abstract: The development of efficient, low-cost, and durable electrocatalysts for sustainable hydrogen production via electrochemical reactions. Here, we report a binary $CoMoO_4/TiO_2$ nanoheterostructure synthesized via a hydrothermal method and analysed as a noble-metal-free electrocatalyst for alkaline HER. The crystal structure, surface morphology, and textural properties of the material were thoroughly investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Characterization of morphology and structure reveals successful incorporation of $CoMoO_4$ into TiO_2, indicating the formation of a stronger interface between the two phases. Electrochemical evaluation in a typical three-electrode system shows the heterostructure outperforms either component alone. A very low overpotential of 142 mV was observed for this nanocomposite, along with a Tafel slope of 132 mV dec^{-1} and a charge transfer resistance (R_{ct}) of 1.06 Ω. The enhanced HER performance is mainly attributed to the synergistic effect at the heterojunction surface, enabled by high charge-transfer efficiency and a high density of electrochemically active sites. Such results suggest that $CoMoO_4/TiO_2$ synthesized via the hydrothermal method is a highly effective alkaline water-splitting electrocatalyst derived from naturally occurring materials.

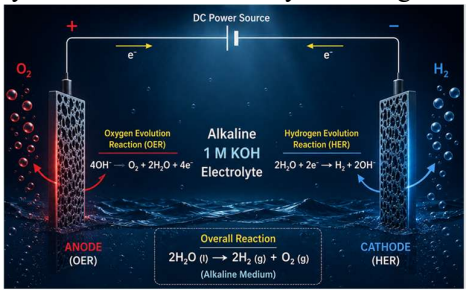

Figure 1. Schematic illustration of alkaline water electrolysis in 1 M KOH electrolyte.

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PP-72

Alcoholysis of furfuryl alcohol using Mo_2C/carbon catalyst

Ramya P*, Cheralathan K. K.

Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India

E-mail: ramya.p2020@vitstudent.ac.in; *Corresponding author: cheralathan.k@vit.ac.in

Abstract: Upgrading biomass-derived molecules into fuels and chemicals is highly desired.[1] In this context, catalytic conversion of furfuryl alcohol, a key molecule obtained from furfural, to get fuel additives, solvents and fine chemicals is a promising approach.[2,3] In the present study, molybdenum carbide (Mo_2C) embedded on carbon was prepared and investigated as the catalyst for alcoholysis of furfuryl alcohol using isopropanol. The catalysts were characterized by X-ray diffraction, N_2 adsorption, FTIR, Raman, FE-SEM, TPD-NH_3, ICP-MS and X-ray photoelectron spectroscopy. The role of adding levulinic acid to glucose during the preparation of carbon (hydrochar) in enhancing the catalyst surface area and improving catalytic activity was investigated. The addition of levulinic acid introduced more functional groups, thereby enhancing the anchoring of the molybdenum precursor and the surface area of the Mo_2C/carbon catalyst. Different reaction parameters such as reaction temperature, reaction time and catalyst loading were varied, and their influence on the alcoholysis reaction was studied. Under optimised conditions, the 20% Mo_2C/Carbon catalyst showed 88% conversion of furfuryl alcohol with 66% and 34% selectivity for isopropyl furfuryl ether and isopropyl levulinate, respectively. The catalyst could be reused for many catalytic cycles.

Keywords: Molybdenum carbide, carbon, hydrochar, furfuryl alcohol, alcoholysis, biomass valorisation.

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PP-73

Electrospun PVDF and ZnO-PVDF composite fibres for wastewater purification

Ritu Purna Sahu
Siksha 'O' Anusandhan, Bhubaneswar, Odisha, India,
email:ritusahu281999@gmail.com

Abstract: The present study investigates the properties and potential applications of electrospun poly(vinylidene fluoride) (PVDF) and ZnO–PVDF composite fibres for water purification. PVDF and ZnO–PVDF composite fibres were fabricated using an electrospinning process, followed by structural and morphological characterization. The incorporation of ZnO particles into the PVDF matrix is investigated to enhance the functional properties of the polymer and facilitate charge generation under thermal stimulation. The elemental composition and surface morphology of the PVDF and ZnO–PVDF fibres were studied. The electrical response of the PVDF and ZnO–PVDF films were evaluated through dielectric permittivity and dielectric loss measurements. The composite shows improved permittivity with low loss at room temperature. The wastewater treatment of the materials was studied to find out the application of these nanofiber composite for water purification. Through the physical separation and catalytic decomposition, PVDF and ZnO composite materials breaks the pollutant's molecule and treat the wastewater.[1] The pyrocatalytic performance of the materials was investigated using methylene blue as an organic pollutant. Under repeated heating-cooling cycles, thermally induced changes in polarization generate surface charges that promote reactions with surrounding water and dissolved oxygen. Reactive species, including hydroxyl and superoxide radicals, contribute to the degradation of the dye molecules. In this work, it has been observed that the maximum methylene blue dye is degraded up to ~ 91 % after 60 heating/cooling cycles. This result demonstrates the potential application of ZnO and PVDF composite fibres as a composite material for water purification.

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PP-74

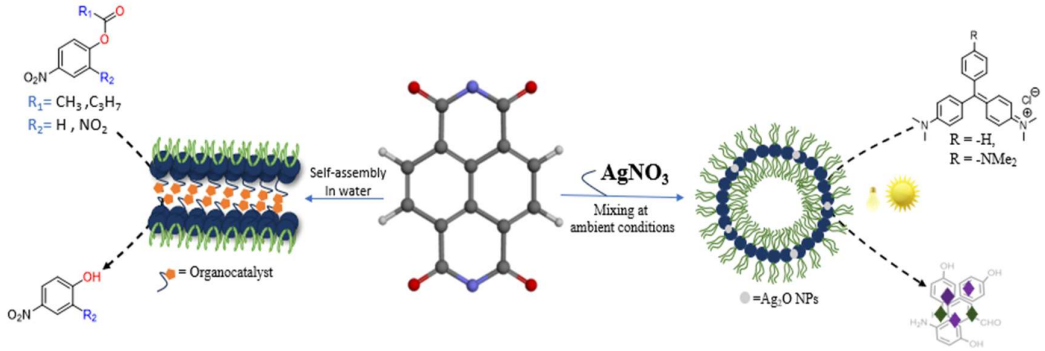
Self-Assembled Naphthalenediimide Nanoreactors for Sustainable Catalysis and Nanomaterial Synthesis

*Rohan Gharad, Chandan Maity**

(Organic) Material Science and Engineering Lab, Department of Chemistry, School of Advanced Science (SAS), Centre for Nanobiotechnology (CNBT), Vellore Institute of Technology (VIT), Vellore campus, Tamil Nadu, India-632014

Email: chandan.maity@vit.ac.in

Abstract: Supramolecular self-assembly provides a powerful strategy for creating organized and confined microenvironments that regulate molecular interactions and enable efficient chemical transformations in water.[1] In this presentation, I will highlight the multifunctionality of naphthalenediimide (NDI)-based supramolecular assemblies as enzyme-mimetic catalysts and nanoscale reactors for sustainable synthesis of Ag_2O nanoparticles. An imidazole-functionalized NDI amphiphile self-assembles into ordered architectures containing hydrophobic pockets and catalytic sites, enabling efficient hydrolysis of 4-nitrophenyl esters and aspirin with Michaelis–Menten kinetics, characteristic of enzyme-like substrate recognition and catalysis.[2] Building on this supramolecular confinement, NDI-based vesicles further serve as nanoreactors for the in-situ synthesis of ultrasmall Ag_2O nanoparticles (~8 nm) under mild aqueous conditions. The resulting NDI/Ag_2O nanohybrid exhibits enhanced visible-light photocatalytic activity, achieving 97% and 90% degradation of malachite green and crystal violet, respectively, with complete degradation of mixed dyes.[3] These findings demonstrate the potential of NDI assemblies as versatile platforms for aqueous catalysis, sustainable nanomaterial synthesis, and environmental remediation.



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PP-75

Porphyrin-Based Catalysts for Sustainable Visible-Light-Assisted Knoevenagel Condensation

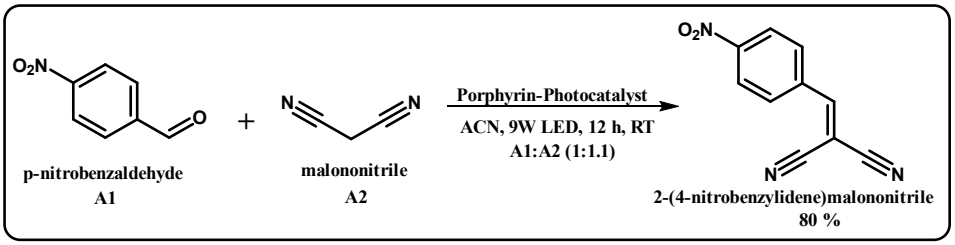
Rushikesh Rajaram Nigade[a], *Kaartik Kalpesh Chandan*[a] and *Dr. Pundlik Rambhau Bhagat*[a]*

[b] Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, India.

* Corresponding author: drprbhagat111@gmail.com, pundlik.rb@vit.ac.in (Pundlik Rambhau Bhagat)

Abstract: In the present study, a porphyrin-based photocatalyst was acquired from 1-(4-formylphenyl)-3-sulfo-1H-benzo[d][1,2,3] triazol-3-ium chloride and pyrrole in acetic acid under reflux conditions. The synthesized photocatalyst was confirmed by using various analytical techniques for structural and physicochemical properties. The photocatalytic performance of the synthesized porphyrin was investigated for the Knoevenagel condensation of aryl aldehydes with active methylene compounds. The protocol represents a versatile and efficient synthetic strategy for construction of C=C bonds to acquire synthetically important alkene derivatives. In this work, the porphyrin photocatalyst was employed under low-power visible-light irradiation (9 W) at room temperature to afford Knoevenagel condensation under mild reaction conditions. The desired alkene product was obtained in good yield of 80% after 12 h of irradiation. The desired product was characterized by proton NMR and GC-MS spectra. Accordingly, the potential of porphyrin-based photocatalyst proved as an environmentally benign approach to the Knoevenagel condensation under visible-light irradiation.

Scheme:



Scheme 1. Synthesis of 2-(4-nitrobenzylidene) malnonitrile

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PP-76

Mechanochemical Solid Solution Formation in Zeolitic Imidazole–Tetrazole Frameworks for Enhanced Oxygen Evolution Reaction

Shafeeq Sarfudeen[1], Sailesh Nithin[2], Sellappan Senthilkumar[3], Harshini Annadata and *Tamas Panda*[4]*

[1] *Vellore Institute of Technology (VIT), Vellore, Tamil Nadu, India, 632014*

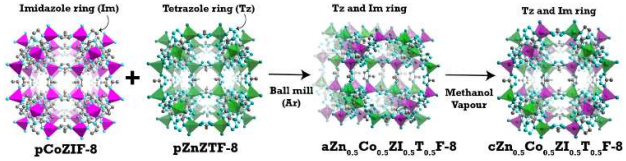
[2] *Vellore Institute of Technology (VIT), Vellore, Tamil Nadu, India, 632014*

[3] *Bhabha Atomic Research Center (BARC), Mumbai, India,40008*

[4] *Vellore Institute of Technology (VIT), Vellore, Tamil Nadu, India, 632014*

Abstract: Investigating heterometallic frameworks with uncoordinated nitrogen sites in zeolitic imidazole–tetrazole frameworks (ZITFs) offers a distinctive strategy to improve electrocatalytic activity. In this study, a solvent-free mechanochemical alloying method is introduced to simultaneously induce Co–Zn metal mixing and imidazole–tetrazole ligand mixing, forming an amorphous solid solution, a$Zn_{0.5}Co_{0.5}$ZITF-8, from ZnZTF-8 and CoZIF-8 under an argon atmosphere. Exposure of this phase to methanol vapor at 25 °C converts it into a crystalline counterpart, c$Zn_{0.5}Co_{0.5}$ZITF-8. Structural and compositional analyses using X-ray absorption spectroscopy, ICP-MS, HAADF-STEM, and FESEM confirm metal–ligand solid solution formation and abundant defect-associated uncoordinated nitrogen sites in the amorphous phase. Owing to its higher active-site density and structural heterogeneity, the amorphous material exhibits superior oxygen evolution reaction performance, with an overpotential of 338 mV and a Tafel slope of 94.8 mV dec^{-1} compared to parent frameworks. Computational hydrogen electrode calculations evaluating *OH, *O, and *OOH intermediates further validate the enhanced activity. This work demonstrates that mechanochemically induced dual solid-solution formation is an effective and sustainable route for designing non-crystalline MOFs with high electrocatalytic efficiency.

Figure/Scheme:



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PP-77

Synthesis of 1,4-Substituted-1,2,3-Triazole by using Fe(II)-Porphyrin Photocatalyst

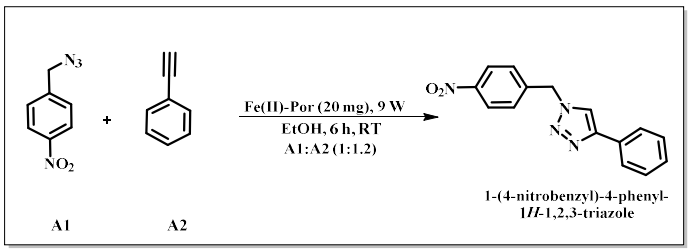
Sakshi Ravindra Giradkar[a] and *Pundlik Rambhau Bhagat*[a]*

[c] Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, India.

*Corresponding author: drprbhagat111@gmail.com, pundlik.rb@vit.ac.in (Pundlik Rambhau Bhagat)

Abstract: In the present study, the Fe(II)-porphyrin complex was synthesized by metalation of the porphyrin macrocycle with ferrous sulfate at 95 °C. The porphyrin macrocycle was prepared through the condensation of 2-formylbenzoic acid with pyrrole in acetic acid (AcOH) under reflux conditions. The photocatalyst was confirmed by the various analytical techniques. The resulting Fe(II)-porphyrin complex was explored for azide–alkyne cycloaddition under irradiation of visible-light. The protocol found environmentally benign alternative to conventional thermal activation methods. The optimized parameters for photocycloaddition of 4-nitrobenzyl azide with phenylacetylene were found to be 20 mg photocatalyst, 2–3 drops of triethylamine (TEA), and 9 W light irradiation in ethanol at room temperature for 6 h. The model reaction afforded the desired 1-(4-nitrobenzyl)-4-phenyl-1H-1,2,3-triazole in 85% yield. The standard parameters were utilized to acquire different derivatives of triazoles with moderate to good yields.

Scheme:



Scheme 1. Synthesis of 1-(4-nitrobenzyl)-4-phenyl-1H-1,2,3-triazole

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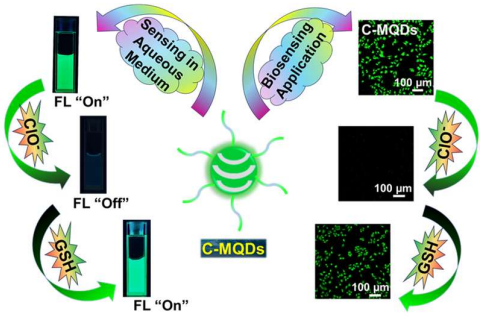
PP-78

Chiral and Bright Green Fluorescent MXene Quantum Dots as "On/Off/On" Nanoprobe for the Selective and Ultrasensitive Detection of Hypochlorite and Glutathione

*Santanu Bera, Evangeline Lawrence, Kamalesh S, Vijay Sithaiyan, Umarfaruk S. Sayyad, Somen Mondal, Anbalagan Moorthy, and Susanta Kumar Bhunia**

[*]Assistant Professor, Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014 Tamil Nadu, India, susanta.bhunia@vit.ac.in

Abstract: MXene quantum dots (MQDs) exhibit excellent optical properties and good biocompatibility, making them promising materials for sensing and biomedical applications. We report the synthesis of bright green emissive chiral MQDs (C-MQDs) with the highest fluorescence quantum yield of 59% by using a simple solvothermal method. The synthesized C-MQDs exhibited a maximum emission at 495 nm upon excitation at 400 nm. Notably, the fluorescence intensity of the C-MQDs was strongly reduced after the addition of hypochlorite (ClO^-) ions. Mechanistic studies indicated that this quenching occurred through a static quenching process, resulting from the formation of a nonfluorescent complex between ClO^- ions and the surface functional groups of the C-MQDs. Surprisingly, the fluorescence was restored after the addition of glutathione (GSH) to the C-MQDs-ClO^- complex, as GSH reduced the ClO^- ions. As a result, the fluorescence "on/off/on" behavior of the C-MQDs was used to detect ClO^- and GSH with very good limit of detection (LOD) as 33 and 50 nM, respectively. Furthermore, the analytes were successfully detected inside living cells, demonstrating the probe's capability for intracellular sensing applications. Moreover, ClO^- ions were detected in real water samples with a very good recovery, even in the presence of other contaminants. These results demonstrate that such a nanoprobe has great potential in therapeutic applications.



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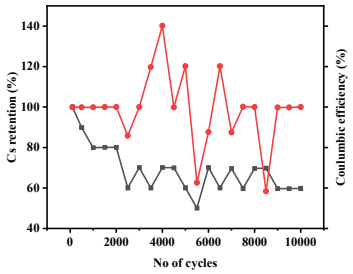
PP-79

Dual-Functional CeO_2-MoS_2-NiO Nanocomposite for Supercapacitor Electrodes and Substituted *N*-heterocycle Synthesis

Ramyashree N[1], *Santhosh G*[2]*
[1]*Department of Chemistry, Christ University, Bengaluru, 560029, India*
[2]*Department of Sciences and Humanities, Christ University, Bengaluru, 560074, India*
**Corresponding author: gsanthosh.2009@gmail.com*

Abstract: In this study, cerium oxide (CeO_2), molybdenum disulfide (MoS_2), and nickel oxide (NiO) were synthesized *via* a co-precipitation method and subsequently integrated through ultrasonication to develop a CeO_2–MoS_2–NiO (CMN) nanocomposite. The structural, morphological, and compositional characteristics of the uncalcined (CMN-U) and calcined (CMN-C) samples were systematically investigated using p-XRD, SEM, EDX, FTIR, BET, TEM, and XPS analyses. Electrochemical investigations demonstrated that the CMN-C electrode exhibited superior charge-storage characteristics, achieving a maximum specific capacity of 268.5 C g^{-1} at a low scan rate and remarkable cycling stability over 10,000 cycles. These results confirm its battery-type charge-storage behavior and enhanced electrochemical kinetics following calcination. In addition, CMN-U and CMN-C were investigated as heterogeneous catalysts for the multicomponent synthesis of substituted 1*H*-tetrazoles, with CMN-C affording yields up to 90%. An asymmetric supercapacitor (AS) device employing CMN-C as the positive electrode exhibited a high specific capacitance of 518 F g^{-1}, a broad operating voltage window, excellent rate capability, and outstanding long-term cycling stability. Overall, the multifunctionality of the CMN-C nanocomposite demonstrates its potential as a sustainable material platform for high-performance energy-storage systems and environmentally benign catalytic applications.

Figure/Scheme: Specific capacitance retention and coulombic efficiency with cycle number for CMN-C



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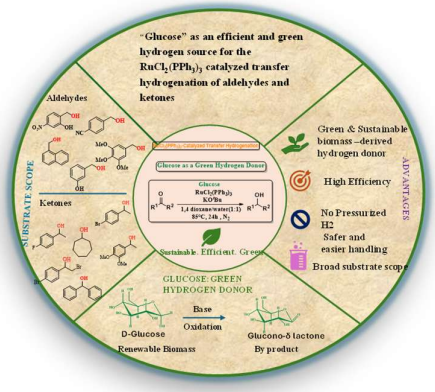
PP-80

GLUCOSE AS AN EFFICIENT AND GREEN HYDROGEN SOURCE FOR $RuCl_2(PPh_3)_3$ CATALYSED TRANSFER HYDROGENATION OF ALDEHYDES AND KETONES

SHAIK ANISHA, *ARUP SINHA**
Research scholar, Department of Chemistry, SAS, Vellore Institute of Technology.
Shaik.anisha2024@vitstudent.ac.in

Abstract: Transfer hydrogenation is an attractive method for reducing aldehydes and ketones without using molecular hydrogen under high pressure. Glucose represents an attractive renewable alternative to conventional hydrogen donors in transfer hydrogenation reactions. Herein, glucose is investigated as a biomass-derived hydrogen source for $RuCl_2(PPh_3)_3$-catalyzed reduction of aldehydes and ketones to the corresponding alcohols. The study examines the relationship between glucose-mediated hydrogen transfer, ruthenium catalyst speciation and carbonyl reduction with product formation and catalyst related species evaluated by the chromatographic and spectroscopic techniques. The findings provide insight into the proposed Ru-mediated hydrogen transfer pathway and highlight the potential of glucose as a sustainable hydrogen donor for the catalytic carbonyl reduction.

Figure/Scheme:



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PP-81

Reduced Graphene Oxide-Supported Zirconium-Nickel Oxide Composite for Efficient Overall Water Splitting

*Sountarya meenal, Stalin Thambusamy**

Department of Industrial Chemistry, Alagappa University, Karaikudi - 630 003, Tamil Nadu, India.

Presenting author E-mail: n.soundharya2019@gmail.com

**Corresponding author E-mail: stalin.t@alagappauniversity.ac.in*

Abstract: A reduced graphene oxide-supported zirconium-nickel oxide (rGO@$ZrNi_4O$) composite was successfully synthesized using a simple hydrothermal method. Structural analyses confirmed the formation of $ZrNi_4O$. The electrocatalytic performance of the rGO@ZrNi4O catalyst was evaluated in a 1.0 M KOH solution, demonstrating excellent performance for the oxygen evolution reaction (OER) with low overpotentials of 270 mV at a current density of 10 mA cm^{-2}. The catalyst exhibited a lower Tafel slope of 157 mV dec^{-1} compared to rGO and $ZrNi_4O$, indicating faster reaction kinetics. The double-layer capacitance (Cdl) value of 15.1 mF cm^{-2} and the lower charge-transfer resistance observed through electrochemical impedance spectroscopy (EIS) confirmed a larger electrochemically active surface area and more efficient electron transfer. Additionally, the catalyst displayed improved hydrogen evolution reaction (HER) activity compared to the individual materials. The alkaline rGO@$ZrNi_4O$‖rGO@$ZrNi_4O$ electrolyzer required a cell voltage of 1.41 V at a current density of 10 mA cm^{-2} and maintained stable performance over 100 hours. The enhanced performance is attributed to the strong interaction between the conductive rGO sheets and the $ZrNi_4O$, which improves electrical conductivity and provides more active sites. Therefore, the rGO@$ZrNi_4O$ composite is a promising, low-cost electrocatalyst for efficient and stable water splitting.

Keywords: reduced graphene oxide, rGO@$ZrNi_4O$, OER, HER, Electrocatalyst, Alkaline electrolyzer

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PP-82

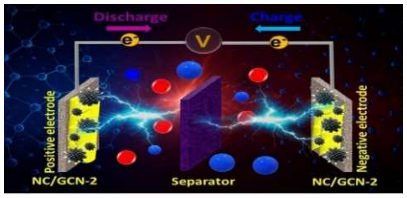
Hydrothermally synthesised synergistic $NiCo_2O_4$/g-C_3N_4 nanocomposite for a highly stable symmetric supercapacitor

D. Subhashini[1], A. Sowmya[1]*

Department of Chemistry, KPR Institute of Engineering and Technology, Coimbatore-641 407, India.

drasowmya@gmail.com

Abstract: The development of electrode materials with high specific capacitance and long-term cycling stability remains a key challenge for advanced supercapacitor applications. In this work, $NiCo_2O_4$/g-C_3N_4 nanocomposite was synthesised via a hydrothermal–calcination method to promote strong interfacial interaction between $NiCo_2O_4$ and g-C_3N_4. The electrochemical performance of the composite electrode was evaluated using cyclic voltammetry, galvanostatic charge–discharge, and electrochemical impedance spectroscopy techniques. In a three-electrode system, the $NiCo_2O_4$/g-C_3N_4 electrode delivered a high specific capacitance of 411.5 F g^{-1} at 1 A g^{-1} and retained 99% of its initial capacitance after 2000 cycles. Furthermore, a symmetric supercapacitor device assembled using identical electrodes achieved an energy density of 36.54 Wh kg^{-1} at a power density of 500 W kg^{-1}. It exhibited 86.36% capacitance retention after 12,000 charge–discharge cycles. These results demonstrate that interfacial engineering of $NiCo_2O_4$ with g-C_3N_4 is an effective strategy for improving the electrochemical performance of supercapacitor electrodes.



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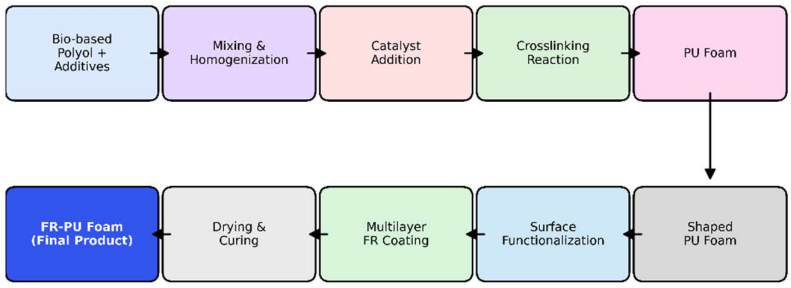
PP-83

Advanced Flame-Retardant Polyurethane Foams: Next-Generation Materials for Multifunctional Performance

*V. Sravani, Indresh Singh, Latha Sinivasan, Rajagopal Desikan, Akella Sivaramakrishna**
*Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology (VIT), Vellore – 632014, Tamil Nadu, India. *E-mail: [asrkrishna@vit.ac.in]*

Abstract: Conventional petroleum-based polyurethane foams (PUFs) are inherently flammable and release toxic combustion by-products, posing severe fire safety hazards across industrial and consumer applications. To overcome these limitations, this study presents a sustainable, bio-derived polyurethane foam engineered via a multilayer surface-coating strategy that simultaneously confers robust flame retardancy, mechanical reinforcement, antibacterial efficacy, and UV-shielding performance. A green PU foam was synthesized from a plant-derived polyol and systematically functionalized using a synergistic combination of an inorganic ceramic additive and a naturally sourced, carbon-rich material. Spectroscopic and structural characterization (FT-IR, XRD, and UV-Vis) confirmed successful, uniform deposition, with the degree of surface modification scaling directly with treatment intensity. Relative to unmodified PU foam, the engineered hybrid foam demonstrated superior mechanical resistance, pronounced antibacterial activity against both Gram-positive and Gram-negative bacterial strains, and exceptional protection against UV-induced photodegradation. Flammability testing (UL-94) revealed a dramatic reduction in burning rate and after-flame duration, completely suppressing the severe melt-drip behavior typical of untreated foams through a robust char-forming barrier mechanism. Overall, this scalable, multifunctional coating approach provides a viable pathway toward high-performance, eco-friendly polyurethane materials for advanced fire safety, healthcare devices, and protective packaging systems.

Figure/Scheme:



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PP-84

Morphology Tuned Viologen-Based Covalent Organic Frameworks: A Fast and Targeted Approach to Eliminate Toxic Organic Pollutants from Water

Pampa Jhariat [1], **Mebin Varghese[1]**, Tamas Panda*[2]

1. Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu-623014, India.

2. Centre for Clean Environment, Vellore Institute of Technology, Vellore, Tamil Nadu-623014, India.

Author E-mail: tamaskumarpanda@vit.ac.in

Abstract: Recent efforts to detoxify contaminated water with various materials have been met with limited success, largely due to insufficient understanding of how material properties affect sorption performance. The application of porous materials with diverse morphologies in water decontamination has been ignored due to synthetic challenges and stability. Here, we report the synthesis of two chemically stable, crystalline viologen-based covalent organic frameworks (vBPDP and vMEL) with distinct morphologies; rod-shaped [vBPDP-8(R) and vMEL-7(R)] and spherical [vBPDP-7(S) and vMEL-8(S)], were achieved by core plane modulations of the monomer (planar vs. nonplanar) and solvent mixture type (polar vs. nonpolar). We employed FESEM and HRTEM imaging of vBPDP at varying time intervals for a comprehensive analysis of the mechanisms of self-assembled morphologies. Further, we compared the adsorption efficiencies of rod- and sphere-shaped vCOFs for removing anionic and neutral dyes from contaminated water. Rod-shaped vBPDP-8(R) and vMEL-7(R) demonstrated superior capture efficiencies than spherical vBPDP-7(S) and vMEL-8(S). vBPDP-8(R) achieved the highest capture of anionic dye-methyl orange (1161.78 mg/g) and neutral dye-fluorescein (1237.40 mg/g). DFT-based analyses (HOMO–LUMO, NBO, NCI and QTAIM) show that vCOFs have much stronger and more uniformly distributed NCIs with anionic (ARS−) and neutral (FL) dyes than with cationic MB+. Compared with vMEL, the donor–acceptor vBPDP shows improved charge-transfer characteristics and stronger binding energies for interaction with ARS− due to an extensive hydrogen-bond network. These results are consistent and explain the experimental results for the adsorption behaviour of vCOFs.This study uniquely explores the creation mechanisms and morphology-dependent performance of self-assembled vCOFs, emphasizing their potential in water treatment and material design.

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PP-85

Borophene Nanosheets Supported Cobalt and Nickel Based Spinal Electrocatalyst for Water Oxidation

Veni Soundra Krishnan,[a] *and Anandhakumar Sukeri*[*a]

[a] Nanoscale Materials Electrochemistry Laboratory, Department of Chemistry
SRM Institute of Science and Technology, Kattankulathur - 603 203
Tamil Nadu, India. *Email: anandhas2@srmist.edu.in

Abstract: Developing highly efficient and durable catalysts for water splitting reactions are essential for sustainable green hydrogen production. Herein, a borophene nanosheets-supported cobalt–nickel oxide spinal catalyst was demonstrated as an efficient water oxidation electrocatalyst, which consists of spherical spinal nanoparticles anchored onto borophene nanosheets (BNS), providing an interconnected heterostructures with abundant accessible active sites and enhanced interfacial charge-transfer properties. The synergistic interaction between the mixed-metal oxides with borophene framework facilitates efficient electron transport and promotes favourable kinetics for water oxidation. Electrochemical results exhibits a low overpotential of ~210 mV to reach the benchmark mark current density of 10 mA/cm^2, with a Tafel slope of 47 mV/dec. Besides, the catalyst also shows an excellent stability over 100 h, which suggests the strong structural and electrochemical stability under prolonged alkaline conditions. Hence, this work demonstrate that integrating the spinel with BNS is an effective strategy for constructing excellent water oxidation performance for clean energy applications.

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PP-86

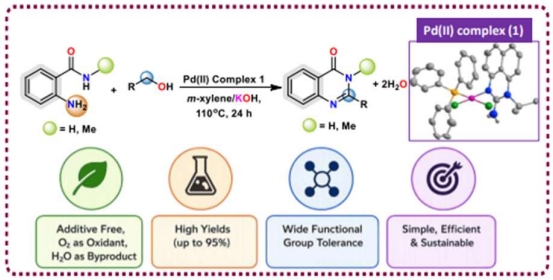
An air tolerant N-heterocyclic imine–Pd (II) catalyst for oxidative dehydrogenative annulation of alcohol towards quinazolinones scaffolds

Aditya L. Shinde[a‡], Preethi Raja[a‡], Priyanka Velmurugan[a], Akash K. Sahoo[a], Manickaraj Meena[a],
Abir Sarbajna[a], Vipin Mishra[a], Tapas Ghatak[a]*
[a] Advanced Catalysis Facility, Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India, Mail ID: tapas.ghatak@vit.ac.in

Abstract: Nitrogen-containing heterocycles[1] are ubiquitous structural motifs in natural products[1], pharmaceuticals[2], and agrochemicals[3]. Among these, quinazolinones have attracted considerable attention because of their diverse biological activities and their presence in numerous bioactive molecules. Despite the availability of several synthetic methods, many protocols rely on stoichiometric reagents, generate undesirable waste, or exhibit limited atom economy[4] .In this work, we describe a catalytic approach to the synthesis of quinazolinones using a newly prepared perimidin-2-imine palladium(II) complex. The air-stable NHI–Pd(II) complex efficiently catalyzes the oxidative dehydrogenative coupling of benzyl alcohols with 2-aminobenzamide or its *N*-methyl analogue to produce a broad range of 2-aryl quinazolin-4(3H)-ones.[5] The reactions proceed under an oxygen atmosphere without additional oxidants, using molecular oxygen as the terminal oxidant. Catalyst loadings as low as 1 mol% provide isolated yields of up to 95%, with water as the only stoichiometric byproduct.

Mechanistic insight was obtained through stoichiometric control experiments, which enabled the isolation and characterization of key intermediates generated from the reaction of benzyl alcohol derivatives with 2-aminobenzamide.[5] These observations are consistent with the proposed catalytic cycle and provide experimental support for the intermediates involved in the transformation. The present method offers an additive-free and atom-economical route to quinazolinones, demonstrating the effectiveness of the NHI–Pd(II) complex for aerobic oxidative dehydrogenative coupling.

Scheme 1: NHI-Pd(II) complex (1) catalyze synthesis of quinazolinone.



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PP-87

An N-Heterocyclic Imine Ligand Platform Enables Base-Minimized Copper-Catalyzed Amination of Aryl Chlorides

Akash Kumar Sahoo, Tapas Ghatak*

Advanced Catalysis Facility, Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, Tamil Nadu, India.
E-mail: tapaschem@gmail.com; tapas.ghatak@vit.ac.in

Abstract: Anilines underpin countless pharmaceuticals, agrochemicals, and polymer precursors, yet their conventional synthesis via nitration and hydrogenation remains a hazardous, poorly selective route that is ill-suited to sensitive functionality. Direct catalytic amination of aryl chlorides with ammonia offers a far cleaner alternative, but every leading Cu-catalyzed system—built on oxalamide, diamine, or phenanthroline ligands remains shackled to large excesses of strong base (1.2–4.5 equiv), a constraint that quietly excludes much of the base-sensitive heterocyclic and electrophilic chemical space central to pharmaceutical synthesis. Here, we break that dependence. By pairing copper with an N-heterocyclic imine (NHI) ligand a scaffold long confined to the exotic world of high-oxidation-state and actinide coordination chemistry, and never before harnessed for 3d transition-metal catalysis, we unlock a mild, non-nucleophilic donor environment that transfers seamlessly to copper. This environment sustains efficient catalysis at low loading and low temperature under dramatically reduced base requirements, even as aqueous ammonia does double duty as both nitrogen source and reaction medium. The resulting catalyst delivers uniformly broad scope across electron-rich, electron-poor, and heteroaromatic aryl chlorides, directly resolving the base-dependence and functional-group limitations that have long constrained Cu-catalyzed chloroarene amination. The NHI ligand and its copper complex were characterized by HRMS, FT-IR, UV-visible spectroscopy, and single-crystal X-ray diffraction, providing compelling structural and spectroscopic confirmation of complex formation. Stoichiometric trapping of key catalytic intermediates further furnishes direct mechanistic evidence for the proposed catalytic cycle. Together, these results establish Cu–NHI complexes as a powerful, underexploited platform for earth-abundant-metal catalysis, charting a practical, atom-economical path from abundant chloroarene feedstocks to functionalized aniline.

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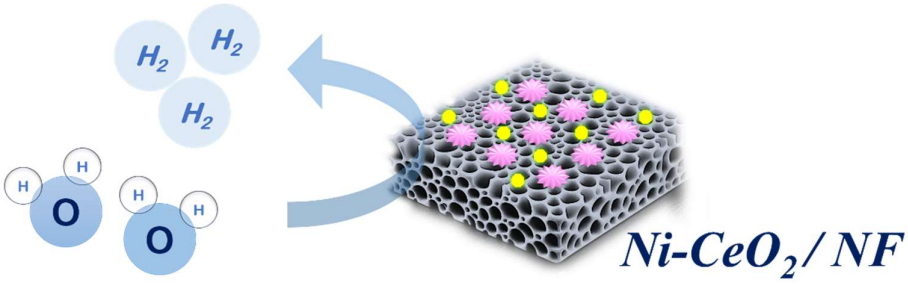
Defect-Engineered Ni-CeO_2 Heterojunctions for Superior Alkaline Hydrogen Production

Tamizharasan B [1], Nasrin Banu G [2], Sandeep Kumar Lakhera [1]*, Neppolian Bernaurdshaw [2]*

1.Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamil Nadu, 603203, India.

2.Energy and Environmental Remediation Laboratory, Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamil Nadu, 603 203, India.

Abstract: The accelerating demand on green energy rapidly increasing due to its zero-carbon emission, in which electrochemical water splitting is a promising avenue for sustainable hydrogen production. Developing low cost and highly effective electrocatalysts for hydrogen evolution reaction (HER) are extremely significant. Here we report an in-situ growth of Nickel-Cerium dioxide catalyst on the surface of nickel foam (Ni-CeO_2/NF) using a simple hydrothermal method. The presence of Ni in the composite accelerated the water dissociation kinetics, whereas CeO_2 provided abundant oxygen vacancies and promoted electron transfer through the reversible Ce^{3+}/Ce^{4+} redox couple. The optimized Ni-CeO_2/NF electrocatalyst exhibits remarkable HER activity in 1 M KOH electrolyte with the overpotential (η) of 139 mV at the current density of 10 mA cm^{-2} and the Tafel slope is 392 $mVdec^{-1}$. Furthermore, the as-prepared electrocatalyst maintained its catalytic performance over a continuous period of 50 h. This study demonstrates that Ni-CeO^2/NF as a promising cost-effective non-noble metal based electrocatalyst for high-performance HER under alkaline conditions.



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