

Day1 – 17-11-2025, Auditorium 1

IL1

Controlling G4 DNA topology with small molecules: towards the development of novel therapeutics

M. Carmen Galan

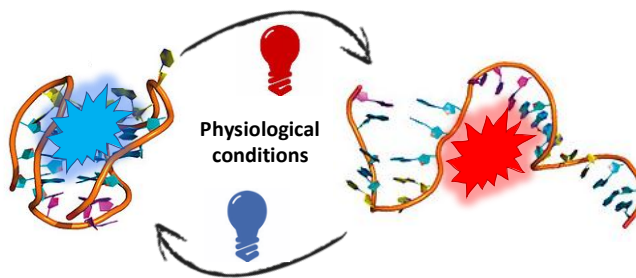
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Abstract:

G-quadruplexes oligonucleotides (G4) are a fascinating class of nucleic acid structures formed from the self-association of guanine-rich sequences. This type of four-stranded structures have found potential applications in biological chemistry and responsive nanotechnology that may be exploited for therapeutic effect. While many examples of ligands that are able to stabilize G4 sequence are reported in the literature, those ligands do not induce reversible and controllable structural perturbations such as the re-folding of the G4 to an alternative topology or the unfolding of the G4 structure through binding modes at physiological pH. In this sense, light offers high spatiotemporal precision for the regulation of oligonucleotide structure and facilitates the investigation of how topological changes influence biological function.¹ During this lecture I will describe recent examples of photoresponsive ligands for G4 DNA regulations developed within our research group. Examples of stiff-stilbene ligands which are capable of unfolding G4 DNA in physiological conditions in a reversible manner² to dithienylethene chromophores or novel diazobenzene molecules with inherently superior photoresponsive properties will be showcased.³



References:

- [1] J. Ramos-Soriano and M. C. Galan, Photoresponsive Control of G-Quadruplex DNA Systems *J. Am. Chem. Soc. Au* **2021**, 1, 10, 1516.
- [2] a) M. P. O'Hagan, S. Haldar, M. Duchi, T. A. A. Oliver, A. J. Mulholland, J. C. Morales, M. C. Galan, A Photoresponsive Stiff-Stilbene Ligand Fuels the Reversible Unfolding of G-Quadruplex DNA, *Angew. Chem. Int. Ed.*, **2019**, 58, 4334-4338. b) M. P. O'Hagan, S. Haldar, J. C. Morales, A. J. Mulholland* and M. C. Galan* "Enhanced sampling molecular dynamics simulations correctly predict the diverse activities of a series of stiff-stilbene G-quadruplex DNA ligands" *Chem. Sci.* **2021**, 12, 1415
- [3] a) M. P. O'Hagan, J. Ramos-Soriano, S. Haldar, J. C. Morales, A. J. Mulholland, M. C. Galan, Visible-Light Photocontrol of G-Quadruplex Ligand Activity: Toggling Binding Mode and Oligonucleotide Folding in Physiological Conditions *Chem. Commun.*, **2020**, 56, 5186; b) J. Ramos-Soriano,* Y.J. Jiang, B. Deng, M. O'Hagan, S. Haldar, A. Grao, S. Oliveira, A. Mulholland, M.C. Galan* "A bridged azobenzene derivative exhibits fully-reversible photocontrolled binding to a G-quadruplex DNA/duplex junction" *JACS Au*, 2025, 5, 3846-3857
- Bio-Sketch of the Speaker

Bio-Sketch of the Speaker

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M. Carmen Galan received her B.S. degree in chemistry from Universidad de Alicante, Spain and an MPhil in Chemistry from the University of Strathclyde (Scotland). She then moved to the USA where she received her Ph.D. in Organic Chemistry from the Complex Carbohydrate Research Center at The University of Georgia, USA, under the supervision of Prof. Geert-Jan Boons, where she carried out research in the field of carbohydrates. She then moved to California to pursue post-doctoral research with Prof. Chi-Huey Wong at The Scripps Research Institute. After that, she continued her post-doctoral training at Massachusetts Institute of Technology with Prof. Sarah O'Connor. Carmen returned to the UK in October 2006 on a lectureship in the School of Chemistry.

She is currently a Professor of Organic and Biological Chemistry in the Chemistry Department at the University of Bristol. Prior to that, she was awarded a series of prestigious fellowships e.g. ERC consolidator grant (2015-2020) and she held an EPSRC Career Acceleration Fellowship (2012-2017) and a Royal Society Dorothy Hodgkin Fellowship (2008-2012).

Her internationally recognized research spans from medicinal chemistry, carbohydrate synthesis, catalysis, functional nanomaterials to biological applications in the areas of cancer, antimicrobials and plant nanobionics. In 2017, she was awarded the RSC Dextra Carbohydrate Chemistry award in recognition of her research into new synthetic methodologies for oligosaccharide synthesis and the development of novel glycoconjugate probes. In 2021 she received the RSC Jeremy Knowles award for the development of bioinspired synthetic probes for the targeting and regulation of cellular processes and in 2022 she was awarded the Spanish Researchers UK (SRUK) Merit award for her contributions to science and the impact of her work to the wider community. In 2025 she received the ACS Melville L. Wolfrom award for her scientific contributions in oligosaccharide chemistry and service to the community and the 2025 Emil Fisher Carbohydrate award.

In addition to her academic duties, She is the Secretary of the International Carbohydrate Committee and Editor-in-Chief of Carbohydrate Research. She is also the co-founder and co-Director of CDotBio Ltd a university of Bristol spin-out.

IL2

Catalyst Engineering for CH Bond Borylation

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Abstract:

The direct C–H bond functionalization using transition metal catalysts is one of the key emergent methods that is currently drawing remarkable attention owing to the rapidly expanding abundant chemical feedstocks to achieve high-valued materials. In this context, catalyst engineering concept through ligand design strategy is one of the most demanding concepts for the direct C–H bond functionalization chemistry. Innovative catalyst design help to deliver the sustainable green chemistry by minimizing extra steps and hazardous toxic materials for a particular reaction. Importantly, direct C-H activation is such innovative idea which originated to eliminates lots of serious problems, now taken a special place towards the sustainable development. Several natural products/chemicals that required multi-step sequences now have been performed with shorter route with improve process through the C-H activation methodology. We have been working in the area of C–H bond activation and borylation chemistry, where site selectivity is primarily controlled by the catalyst engineering concept. In this talk, I will briefly discuss some of our efforts regarding the catalyst engineering concept for the direct CH bond borylation.

References:

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Buddhadeb Chattopadhyay received his M.Sc. in Chemistry from Visva-Bharati University, India, in 2003 and Ph.D. in 2009 from the University of Kalyani with Professor K. C. Majumdar. Following his doctoral studies, he spent nearly six years as postdoctoral research associate—first with Professor Vladimir Gevorgyan at the University of Illinois at Chicago (USA), and later with Professor Milton R. Smith III at Michigan State University, Michigan (USA). In August 2014, he started his independent academic career at the Centre of Biomedical Research (CBMR) in Lucknow, India. Before joining the Indian Institute of Science Education and Research Pune (IISER Pune), Buddhadeb served for more than ten years at the Centre of Biomedical Research (CBMR), Lucknow, in the positions of Assistant Professor, Associate Professor and Additional Professor. Since January 2025, he has been serving as an Associate Professor in the Department of Chemistry at the Indian Institute of Science Education and Research (IISER), Pune.

His research interest includes the catalyst/ligand engineering for the C–H bond activation/functionalization, especially C–H bond borylations of organic molecules and metal-nitrene/carbene chemistry via metalloradical catalysis by means of denitrogenative transformations to make high-valued nitrogen heterocycles.

Dr. Chattopadhyay is a Fellow of the Royal Society of Chemistry, London, UK (FRSC), Fellow of the National Academy of Sciences (FNASc). Dr. Chattopadhyay has been serving as Associate Editor, Organic Chemistry Frontiers (OCF), RSC.

IL3

Design of High-Performance Metal Nanostructured Catalysts for Sustainable Molecular Transformations

Takato Mitsudome

Osaka University, Japan

Abstract

Our research focuses on the design of high-performance metal nanoparticle catalysts that enable green and sustainable molecular transformations under liquid-phase conditions [1]. Our ligand-based design concept applies to both metal oxides and phosphorus, which function as ligands that finely tune the local electronic and coordination environment of metal centers. Metal oxides as secondary components create precisely engineered metal–oxide interfaces, where oxide ligands cooperate with active metal centers to promote substrate activation and achieve outstanding catalytic efficiency. In metal phosphides, phosphorus exerts a strong ligand effect that modulates the electronic structure, resulting in catalysts with remarkable activity and durability. By controlling these ligand–metal interactions at the nanoscale, we achieve catalytic activities and selectivities that surpass those of conventional catalysts in key transformations, including O₂-based oxidations and selective hydrogenations. This design strategy provides general guidelines for the creation of durable and highly active catalysts, contributing to the advancement of sustainable chemical manufacturing.

References:

[1] T. Mitsudome et al, *J. Am. Chem. Soc.*, **2025**, *147*, 14326; *Small*, **2025**, *21*, 2412217; *Nat. Commun.*, **2023**, *14*, 5959; *ACS Catal.*, **2023**, *13*, 5744; *JACS Au*, **2022**, *2*, 419; *JACS Au*, **2021**, *ACS Catal.*, **2021**, *11*, 750; *Chem. Sci.*, **2020**, *11*, 6682; *ACS Catal.*, **2020**, *10*, 4261. *Angew. Chem. Int. Ed.*, **2017**, *56*, 9381. *J. Am. Chem. Soc.*, **2015**, *137*, 13452; *Angew. Chem. Int. Ed.*, **2014**, *53*, 8348; *Angew. Chem. Int. Ed.*, **2013**, *52*, 1481.

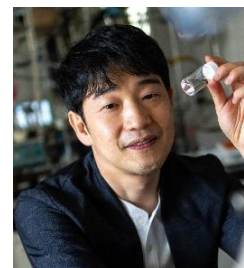
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Research Career

Takato Mitsudome received his Ph.D. (2006) in Engineering from Osaka University under the supervision of Prof. Kiyotomi Kaneda. In 2007, he joined the same university as an Assistant Professor in the Graduate School of Engineering Science, working with Profs. Kiyotomi Kaneda and Koichiro Jitsukawa. He was promoted to Associate Professor in 2016.

His research focuses on the design and development of nano-structured heterogeneous catalysts, aiming at environmentally benign and selective molecular transformations. He has authored over 150 peer-reviewed papers in high-impact journals

Research Interest

- Development of heterogeneous catalysts for green molecular transformations
- Design of non-precious metal nanoparticle catalysts (Fe, Co, Ni, Mn) for liquid-phase hydrogenation and reductive transformations
- Synthesis and catalysis of transition metal phosphides, carbides, and borides as sustainable catalytic materials
- Elucidation of structure–activity relationships through advanced characterization

Awards and Recognitions

17th Green & Sustainable Chemistry (GSC) Encouragement Award, Japan Association for Chemical Innovation

Osaka University Award (Young Professor Section)

Catalysis Society of Japan Award for Young Researchers

Young Scientist Award, 15th International Congress on Catalysis

Publications in Journals & Patents

Peer-reviewed papers: 150+

Patents: 20+

Details of projects handled

National and international research projects: 15+ (including JSPS KAKENHI, JST-CREST, and international collaborations with IIT Hyderabad, CNRS, and TU Wien)

Technology development/ Initiation

Initiation of Osaka University–Zeon Collaborative Research Chair on Advanced Catalysis for Carbon Neutrality (2023–present)

IL4

Catalytic Upgrading of carbon dioxide

Sebastian Wohlrab

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Abstract:

To address the growing demand for sustainable carbon utilization, our research focuses on the development of catalytic processes that enable the direct conversion of CO₂ into valuable chemicals and fuels. Particular emphasis is placed on process intensification through the integration of membrane technologies, reaction coupling, and data-driven process optimization. The direct synthesis of methanol from CO₂ is examined from a technological point of view and the usefulness of process-intensifying methods, such as membrane technologies, or an upstream reverse water-gas shift reaction is discussed. Different methanol catalysts are compared with each other, the conversion-selectivity behaviour is kinetically evaluated and conclusions are drawn for a future technical design. To maximise the conversion of the reactants, we are therefore developing a pilot-scale cycle operation with recirculation of unreacted gases. Furthermore, the release of the inherent energy of methanol with regard to the methanol fuel cell and, alternatively, the low-temperature reforming with downstream gas purification for conventional fuel cell application is examined.

Biomethane, obtained from the fermentation of biomass, can be seen as enriched carbon source of a CO₂ capture from the air via plants. Direct conversion on site of production into a transportable value product would be of great interest in terms of a circular carbon economy. Formaldehyde represents one of the key intermediates in chemical industry. The conventional technical three step process via synthesis gas and methanol is unrealistic to establish around decentralized biogas plants. A direct route would provide enormous savings in energy and investment costs. Herein, we report the influence of single reaction parameters on the selective oxidation of methane with air over an in situ prepared VO_x/silica catalysts with water being identified as key factor for achieving high formaldehyde selectivity and space time yield (> 15 kgH₂CO kg_{cat} h⁻¹). For this purpose, artificial neural network modelling was performed and used for the prediction of methane conversion and formaldehyde selectivity for different input parameters over a wide range.

In summary, these studies provide important insights into efficient catalytic systems and process concepts that contribute to closing the carbon cycle for a sustainable chemical industry.

Bio-Sketch of the Speaker

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Sebastian Wohlrab obtained his PhD at the Max Planck Institute of Colloids and Interfaces under the supervision of Prof. Markus Antonietti in 2004, after completing his studies in chemistry at the Technical University of Dresden in 2000. Following his doctoral research, he joined the group of Prof. Stefan Kaskel at TU Dresden as a postdoctoral researcher, where he focused on functional porous materials. From 2006 to 2008, he worked as a scientist at the Federal Institute for Materials Research and Testing (BAM) in Berlin. In 2008, Sebastian became Group Leader of “Inorganic Functional Materials” at the Leibniz Institute for Catalysis (LIKAT). He advanced to Junior Research Group Leader in 2011 and was appointed Head of the Department “Heterogeneous Catalytic Processes” in 2017. His research centers on materials and membranes for selective adsorption and mass separation, membrane reactors for CO₂ hydrogenation, and catalyst development for sustainable and exhaust gas processes. Further interests include the use of low-cost raw materials for large-scale catalytic applications, technical upscaling of catalyst syntheses, and modeling of material properties. Sebastian has authored over 160 scientific papers and holds several patents. He has successfully managed more than 30 research projects and initiated four technology transfers to industry.

IL5

Hydrogen-Bond-Mediated Aglycone Delivery

Alexei V. Demchenko, PhD

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3501 Laclede Ave, St. Louis, Missouri 63103, USA

Abstract:

Although carbohydrates are desirable for the pharmaceutical and biomedical communities, these molecules are very challenging targets for chemists because of the need for functionalization, protecting and leaving group manipulations, controlling anomeric stereoselectivity, separation, and analysis. The development of stereocontrolled methods for the synthesis of building blocks,^[1] chemical glycosylation,^[2-3] and glycan assembly^[4] represent demanding areas of research. At the core of this presentation is the development of H-bond-mediated Aglycone Delivery (HAD) method for stereocontrolled glycosylation and the synthesis of glycans. In the HAD reaction, the glycosyl acceptor (aglycone) forms an H-bond with the nitrogen of the picoloyl (Pico) protecting group on the glycosyl donor. Upon the leaving group activation, the acceptor is delivered to form the glycosidic bond with high *syn*-selectivity in respect to the remote Pico group.^[5]

The HAD reaction has been successfully applied to α -glucosylation with 4-Pico donor,^[5] β -gluco with 3-Pico^[6-7] or 6-Pico donor,^[8] β -manno with 3-Pico and/or 6-Pico donors,^[9] and these methods were applied to the synthesis of challenging α -glucans^[10] and β -mannans.^[9, 11] We have also introduced a catalytic method for chemoselective removal of Pico with FeCl₃ in the presence of all other common protecting groups.^[12] More recently, the HAD reaction was applied to glycosidation of mannosamine (ManNAc),^[13] mannuronic acid (ManA),^[11] and ManNAcA^[14] donors. The effectiveness of methods developed will be illustrated by the synthesis of glycopharmaceuticals derived from *S. pneumonia* capsular polysaccharide type 4 (CP4),^[13] β -(1 \rightarrow 3)-linked ManA glycan,^[11] and *Staph. aureus* CP8.^[14]

References

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- [2] S. S. Nigudkar and A. V. Demchenko, *Chem. Sci.* **2015**, *6*, 2687–2704.
- [3] Y. Singh, S. Geringer and A. V. Demchenko, *Chem. Rev.* **2022**, *122*, 11701-11758.
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- [13] C. Alex, S. Visansirikul and A. V. Demchenko, *Org. Biomol. Chem.* **2020**, *18*, 6682-6695.
- [14] C. Alex and A. V. Demchenko, *J. Org. Chem.* **2022**, *87*, 271-280.

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Research Career

2021 - Professor and Chair, Department of Chemistry, Saint Louis University, USA

2014 - 2021 Curators' Distinguished Professor (Emeritus from 01/2023), UM – St. Louis, USA
2011 - 2014 Professor of Chemistry and Biochemistry, UM – St. Louis, USA
2007 - 2011 Associate Professor and Director of Graduate Studies, UM – St. Louis, USA
2001 - 2007 Assistant Professor of Chemistry and Biochemistry, UM – St. Louis, USA
1998 - 2001 Research Associate (Boons), Complex Carbohydrate Research Center, Georgia, USA
1995 - 1998 BBSRC Post-Doctoral Research Fellow (Boons), University of Birmingham, UK
1993 - 1995 Research Associate (Kochetkov), Zelinsky Institute of Organic Chemistry, Moscow, Russia
1988 - 1993 Ph.D. in Organic Chemistry (Kochetkov), Zelinsky Institute of Organic Chemistry, Russia
1982 - 1988 M.S. in Chemical Engineering, Mendeleev University of Chemical Technology of Russia

Research Interest

- Streamlined synthesis of regioselectively protected carbohydrate building blocks
- Novel glycosylation reactions. Stereocontrol and mechanism of chemical glycosylation
- Expeditious strategies for the synthesis of complex oligosaccharides and glycoconjugates
- Synthetic glycopharmaeaceuticals (anti-cancer, anti-bacterial, anti-septic, etc.)
- Human milk oligosaccharides and other food additives and ingredients
- Solid phase and surface chemistry: application to automated glycan synthesis

Awards and Recognitions

2025 Fellow of the American Chemical Society (ACSF)
2024 The Midwest Award, American Chemical Society (ACS), St. Louis Section
2024 The Wolfrom Award, ACS, Division of Carbohydrate Chemistry and Chemical Glycobiology
2022 Fellow of the Saint Louis University Research Institute
2020 Co-Investigators of the Year Award (with K. J. Stine), UM – St. Louis Office of Research
2020 Outstanding Scientists Awards - Fellows Award, Academy of Science - St. Louis
2020 Fellow of the Academy of Science – St. Louis
2020 - 2021 Chair, Division of Carbohydrate Chemistry and Chemical Glycobiology, ACS
2019 - The National Representative of the USA for the International Carbohydrate Organization
2019 - President of the U.S. Advisory Committee for the International Carbohydrate Symposia
2017 Senior Investigator of the Year Award, UM – St. Louis, Office of Research
2015 Chair, Gordon Research Conference on Carbohydrates
2014 St. Louis Award, ACS, St. Louis Section
2013 Chancellor's Award for Excellence in Research and Creativity, UM – St. Louis
2012 - 2021 Associate Editor, Journal of Carbohydrate Chemistry
2007 New Investigator Award, ACS, Division of Carbohydrate Chemistry
2005 CAREER Award, National Science Foundation

Publications in Journals & Patents - 240

OL1

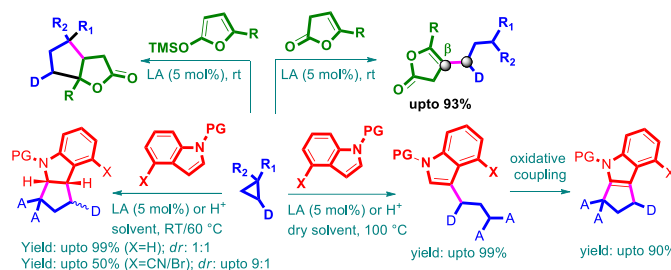
Exploring reactivity of deconjugated butenolides or indoles towards donor-acceptor cyclopropane under catalytic conditions

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Abstract:

Catalytic conversion of renewable biomass into fuel and other valuable chemicals are focused area of modern research.[1] Among them, α -angelica lactone, which is readily available from levulinic acid by intramolecular dehydration, has attracted extensive attention[2] as its butenolide variant. This is due to its potential application in the construction of γ -substituted butenolides natural products and biologically active molecules. Moreover α -angelica lactone is synthetically useful as a nucleophile and it has been exploited in many reaction such as Michael addition, Morita-Baylis-Hillman and Pd-catalyzed cross-coupling reaction etc. to access useful compounds.[3] *On the other hand, cyclopropanes are essential building blocks in organic chemistry due to their unique reactivity and strained structure. The incorporation of donor and acceptor group at vicinal position generates the “push-pull” effect that has been synthetically exploited to access 1,3-functionalized compounds including annulated products.[4] During the reaction initial ring-opened products often undergoes annulations by suitably positioning of complimentary functionality. Taking advantage of this unique reactivity pattern, our research group is involved in developing methods, under thermal, photolytic reaction conditions, to access various indole or lactone based scaffolds of medicinal importance.[5,6] My talk will encompass discussion on some of our recent efforts to develop organic transformations involving donor-acceptor cyclopropane (DAC) and α -angelica lactone or indole derivatives.*



Scheme 1. Reaction of deconjugated butenolides or indoles towards DAC.

References:

- [1] (a) K. Krieger, *Nature* **2014**, *508*, 448-449; (b) J. J. Bozell, *Science* **2010**, *329*, 522.
- [2] (a) M. Besson, P. Gallezot, C. Pinel, *Chem. Rev.* **2014**, *114*, 1827.
- [3] A. Choudhury, S. Mukherjee, *Chem. Soc. Rev.* **2020**, *49*, 67.
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- [5] K. Singha; D. Mallick and K. Ghosh*; (*manuscript submitted*).
- [6] K. Singha; P. Mandal and K. Ghosh*; (*manuscript submitted*)

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Research Career

Ph.D. (2003-2009) from IIT Kanpur (under the supervision of Prof. M K Ghorai)
Post doc: (2010-2011) Purdue University (with Prof. Arun K Ghosh)
Post doc: (2011-2012) IACS, Kolkata (with Prof. A Sarkar)
British Council Fellow (Oct. 2011-Dec. 2011) University of Nottingham [with Prof. S. Woodward]
deputed from IACS, Kolkata
Principal Investigator (2012- April 2013) at Biocon Bristol-Myers Squibb R & D Centre (BBRC), Bangalore
Fast Track Young Scientist (July 2013-Oct. 2013) IIT Kharagpur (with Prof. Amit Basak)
Assistant Professor (Nov. 2013-present) Department of Chemistry, Presidency University, Kolkata

Research Interest

Sustainable Organic Synthesis, Asymmetric Catalysis, Medicinal Chemistry

Publications in Journals & Patents

15

Details of Project Handled

3

OL2

Developing Green Synthetic Methodologies to Access Marketed Drug, Drug Analogues, and Anti-Cancer Agents

Dr. Tanmay Chatterjee

Associate Professor, Department of Chemistry, BITS Pilani, Hyderabad Campus, Jawahar Nagar, Kapra Mandal, Telangana-500078 India.

Abstract:

Sustainability serves as a benchmark for the advancement of contemporary society, and within the realm of chemistry, it can be realized through the implementation of green chemistry principles [1]. This has prompted both industry and academia to pursue sustainable development in the field of chemistry [2]. The development of environmentally friendly and economically viable synthetic methods for producing commercially available pharmaceuticals, their analogs, and innovative drug compounds is a top priority within the pharmaceutical sector [3]. In this lecture, I shall talk about our strategies in developing green and sustainable synthetic methods to access a marketed drug such as tamoxifen, a top-selling anti-breast cancer drug worldwide, some novel drug analogues, and also a new and novel class of molecules and their anti-cancer activities. In particular, we developed a 100% atom-economic and highly regio- and stereoselective iodosulfenylation of alkynes for the synthesis of (*E*)- β -iodoalkenyl sulfides and the utility of the developed green synthetic method was demonstrated by synthesizing a marketed drug, tamoxifen *via* the synthetic diversification of a synthesized product in two steps [4]. We also developed a solvent (HFIP) mediated highly chemo-, regio- and stereoselective hydrofunctionalization of ynamides [5,6], a special kind of alkynes and also demonstrated the utility of the protocol in accessing novel drug analogues, *i.e.*, stereodefined trisubstituted alkenes bearing two different drugs or one drug and one natural product on the same carbon. In another project, we developed a novel synthetic strategy, *i.e.*, metal-free, cascade regio- and stereoselective trifluormethyloximation, cyclization, and elimination strategy with readily available α,β -unsaturated carbonyl compounds to access a wide variety of pharmaceutically potential heteroaromatics, *i.e.*, 4-(trifluoromethyl)isoxazoles, and evaluated their anti-cancer activities, which revealed the importance of a -CF₃ functional group on the 4th position of isoxazole in enhancing their anti-cancer activities [7-9].

References

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Bio-Sketch of the Speaker

Dr. Tanmay Chatterjee

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Dr. Tanmay Chatterjee obtained an M. Sc degree in Chemistry from the Indian Institute of Technology, Delhi (IIT Delhi), India in 2009. He received a Ph.D. degree in organic chemistry in 2014 from the Indian Association for the Cultivation of Science (IACS), Kolkata (the degree was awarded by Jadavpur University) for his research work on green synthesis using benign solvents, reagents, and catalysts under the supervision of Prof. Brindaban C. Ranu. Then he moved to South Korea and worked with Prof. E. J. Cho on visible-light photocatalysis during 2014–2017 at Hanyang University as a postdoctoral fellow (2014 – 2015) and at Chung-Ang University as a research professor (2015 – 2017), respectively.

He returned to India and started his independent career as an Assistant Professor at Birla Institute of Technology and Science, Pilani (BITS-Pilani), Hyderabad Campus in 2018. Currently, he is working as an Associate Professor. His research interests include the development of green organic synthetic methodologies by iodine-catalysis, visible-light photocatalysis, electrochemical organic transformations, solvent-mediated or controlled organic transformations, and metal-free reactions in water with an emphasis on the development of greener synthetic methodologies. So far, Dr. Chatterjee has authored/co-authored 61 papers published in reputed international journals, 3 book chapters and 4 patents, which fetched >2600 citations with an H-index of 29.

Dr. Chatterjee has been serving as an editorial board member of a Scopus-indexed international journal, *Current Green Chemistry* (Impact factor: 1.7) of Bentham Science Publishers, and also as a reviewer of various reputed international journals such as *Green Chem.*, *Org. Lett.*, *J. Org. Chem.*, *Chem. Commun.*, *Adv. Synth. Catal.*, *Org. Chem. Front.*, *Org. Biomol. Chem.*, *Eur. J. Org. Chem.*, *Chem. Asian J.*, *Asian J. Org. Chem.*, *New J. Chem.*, *RSC Adv.*, *Synthesis*, *Synlett*, *ChemistrySelect*, *ChemistryOpen*, *J. Fluor. Chem.* etc since last 7 years. Recently, Dr. Chatterjee has received the prestigious “**Thieme Chemistry Journals Award 2025**”. Last year, he was recognized as an “**Emerging Investigator: 2024**”, by the prestigious journal *Chemical Communications*, and was also elected as “**Associate Fellow of Telangana Academy of Sciences (AFTAS)**”. Dr. Chatterjee received the “**Best Researcher Award**” in the International Scientist Awards on Engineering, Science, and Medicine, held on 12th November 2021 in Chennai, India, organized by the VDGOD professional association.

Furthermore, under his guidance, 1 student has been awarded a Ph.D. degree, and he is currently supervising 8 research fellows in their pursuit of Ph.D. degrees.

SL1

Transition Metal Catalysed Insertion of Diazoquinones

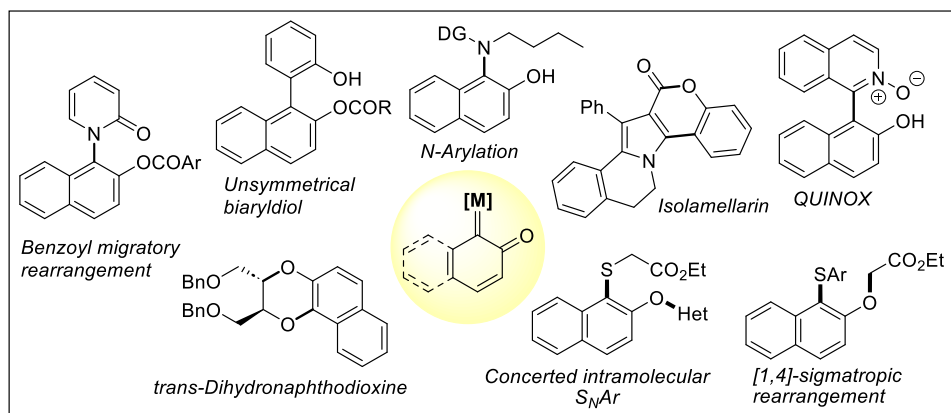
Rajarshi Samanta

Department of Chemistry, Indian Institute of Technology Kharagpur, India

Email: rsamanta@chem.iitkgp.ac.in

Abstract:

The diazo quinone or quinone diazide compounds have been recently explored to introduce phenol/naphthol moieties into the hydrocarbons and hetero atom-containing molecules under transition metal catalysis.¹ The reactions proceed via insertion or migratory insertion of quinoid carbenes into C–H/X–H bonds. In this presentation, the racemic synthesis of phosphine ligands like QUINAP, METHOX, PINAP, and PHENAP and the synthesis of isolamellarin natural products using the migratory insertion of quinoid carbene *via* C–C bond-forming reactions will be explained.^{2,3} Next, *N*-arylation of electron-deficient systems will be discussed.^{4,5} Further, the sigmatropic rearrangement with corresponding sulphur ylides will be illuminated.⁶ Moreover, the insertion of quinoid carbenes into *cis*-epoxides will be discussed with mechanistic details.⁷ Finally, the synthesis of unsymmetrical biaryl diol from enaminone *via* C–C bond activation will be explained.⁸



Scheme 1: Synthetic strategies using quinoid carbene

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Bio-Sketch of the Speaker

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Rajarshi Samanta did his bachelor's (2002) and master's (2004) from Jadavpur University, Kolkata. He received his PhD from the Indian Institute of Chemical Technology, Hyderabad, in 2010 under the supervision of Prof. Tushar Kanti Chakraborty. Subsequently, he moved to the Max Planck Institute of Molecular Physiology, Dortmund, Germany, for his postdoctoral work under Prof. Andrey P. Antonchick as a Max-Planck postdoctoral researcher. Then, he joined the Indian Institute of Technology, Kharagpur, as an assistant professor in September 2013. Currently, he has been an associate professor in the same institute since August 2019. He has been an editorial board member of *Tetrahedron* and *Tetrahedron Letters* since 2024. He received the Chemical Research Society (CRSI) bronze medal (2026), Chirantan Rasayan Sanstha (CRS) silver medal (2025), *Thieme Chemistry Journal Award* (2023), *Associateship for the Indian Academy of Sciences* (2019-2022), and was selected as an *Emerging Investigator* in the *New Journal of Chemistry* (2021). His current research interests are (I) Straightforward synthesis of heterobiaryls and natural products using metal-carbenes and nitrenes (II) Development of macrocyclization methods using metal-carbenes (III) Step-economic construction of nitrogen-containing extended conjugated systems and studying their photophysical properties.

SL2

Beyond the Single Catalyst: Transition Metals in Combined Catalysis

Shikha Gandhi^{1*}¹ Department of Chemical Sciences, Indian Institute of Science Education and Research
Berhampur, Berhampur, Odisha 760010, India.**Abstract:**

Transition metals are the most commonly used catalysts in organic synthesis. Over the last two decades, the combined use of transition metal (TM) catalysts with other catalysts has gained momentum. One excellent application is the combination of palladium or rhodium catalysts with Brønsted acid (HX) catalysts for the direct allylation of nucleophiles with alkynes. This approach is completely atom-economical and offers a great alternative to the 'Tsuji-Trost allylations'. This talk will disclose our results on the Pd/HX co-catalysed intramolecular allylations of nucleophiles with alkynes. An interesting extension of this reaction to the skipped enynes has enabled us to directly access a [3+3]-annulated product with a bis-nucleophile, in a completely atom-economical manner. Our recent results on the expansion of these allylations to the diastereoselective synthesis of 1,3-oxazolidines will also be discussed.

A synergistic combination of N-heterocyclic carbenes with transition metal catalysts is yet another emerging, powerful strategy for tackling challenging transformations. This talk will also disclose the results of our efforts to directly access allyl esters from aldehydes and Morita-Baylis-Hillman carbonates using NHC/TM synergistic catalysis under aerobic conditions. I will also present our recently developed route to access β , γ -unsaturated ketones under inert conditions from the same starting materials.

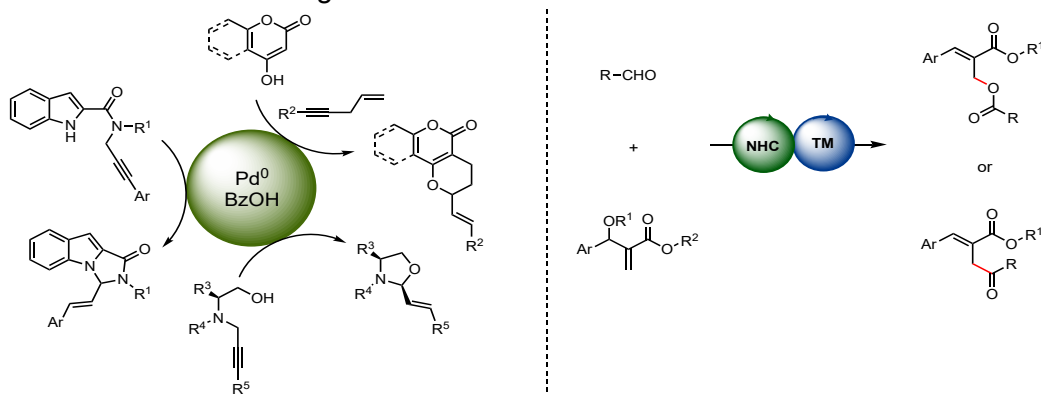


Figure. Pd/Brønsted acid co-catalysed propargylic C-H activations, and NHC/TM synergistically catalysed allylations

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Research Career

Shikha got her M.Sc. degree from Panjab University, Chandigarh, in 2004. She subsequently joined the group of Prof. Vinod K. Singh at IIT Kanpur and graduated with a doctoral degree in 2009. She then moved to the Max Planck Institute for Coal Research, Germany, as a postdoctoral researcher in the group of Prof. Benjamin List. After a brief stint in industry, she began her independent career at IISER Berhampur in 2017. She is currently an Associate Professor at the same institute.

Research Interest

The research in Shikha's is focused on '*catalysis*', exploring the areas of transition metal, organocatalysis, and synergistic catalysis to contribute to the development of processes that are scalable, highly efficient from the point of view of atom economy, and environmentally benign. The group has been actively working on the applications of combined Palladium and Brønsted acid catalysis for propargylic C-H activation. A recent expansion of this catalysis to skipped enynes has led to an exciting [3+3]-annulation with a bisnucleophile, triggering our interest in atom-economical annulations. The team is also active in the relatively underexplored area of synergistic catalysis involving N-heterocyclic carbenes (NHCs) and transition metals. NHCs are additionally explored as organocatalysts by the team. The group's interest also lies in developing asymmetric catalysis with chiral NHCs, leading to enantioselective synthesis of important molecules.

Award and Recognition

Alexander von Humboldt fellowship for post-doctoral research (2010-2012)
Thieme Chemistry Journal Award (2019)

Publications in Journal and Patents

14

Details of Project Handled

01

SL3

Dual Facets of S_N2' Reaction of *gem*-Dichlorocyclobutenones**Basudev Sahoo***

Institute School of Chemistry, Indian Institute of Science Education and Research
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Abstract:

gem-Dichlorocyclobutenones constitute a unique class of compounds, featuring both α,β -unsaturated ketone and allylic dichloride electrophilic motifs embedded within a highly strained four-membered ring.^[1] Relying on the photochemical ring opening,^[2] it was vastly explored in cycloaddition chemistry. However, nucleophilic allylic substitution (S_N2') has sporadically been studied.^[3-5] Recently, organometallic (Zn, Cu) reagents participated in S_N2' based C-C bond formation at low temperature in the presence of transition metal catalysts and suitable ligand systems. Catalytic arylation and alkenylation of *gem*-dichlorocyclobutenones were successfully achieved, employing aryl- and alkenylzinc reagents.^[3,4] A S_N2' allylation of *gem*-dichlorocyclobutenones was reported with organocopper intermediates that are catalytically generated in situ from reactive allenes.^[5] Considering the limitations of metal-catalyzed methods, we have disclosed a unique complementary radical chemistry approach for S_N2' -type alkylation of *gem*-dichlorocyclobutenones with easily accessible and bench-stable C-centered radical precursors under photocatalysis (Fig. 1).^[6-7] This strategy establishes a versatile platform for engaging diverse non-nucleophilic radical progenitors, underscoring radical activation mode for S_N2' -type functionalization of *gem*-dichlorocyclobutenones.

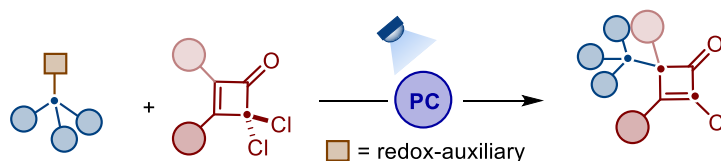


Fig. 1: S_N2' -type alkylation of *gem*-dichlorocyclobutenones.

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- [7] P. P. Mondal, S. Das *et al.*, Manuscript (in preparation).

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Research Career

- Associate Professor (02/2025-present): School of Chemistry, Indian Institute of Science Education and Research (IISER) Thiruvananthapuram, Kerala, India
- Assistant Professor (03/2020-01/2025): School of Chemistry, Indian Institute of Science Education and Research (IISER) Thiruvananthapuram, Kerala, India
- Marie Curie Postdoctoral Fellow (07/2018-02/2020): Institute of Chemical Research of Catalonia (ICIQ) Tarragona, Spain (Supervisor: Prof. Ruben Martin)
- Leibniz Postdoctoral Fellow (10/2015-06/2018): Leibniz-Institute for Catalysis (LIKAT), Rostock, Germany (Supervisor: Prof. Matthias Beller)
- PhD (10/2011 - 08/2015): Westfälische Wilhelms-Universität (WWU) Münster, Germany (Supervisor: Prof. Frank Glorius)

Research Interest

Organic Synthesis: Transition Metal Catalysis and Visible Light Photocatalysis

Award and Recognition

Thieme Chemistry Journals Award from Thieme Verlag (2022)

Member of Early Career Advisory Board (ECAB) of ChemCatChem (2025-present)

Publications in Journal and Patents

Total Publications = 45

Details of Project Handled

3

SL4

Leveraging Unique Reactivity of Sulfonyl Allenes to Construct 'S' Containing Diverse Organic Scaffolds

Dr. Aslam C. Shaikh*

Department of Chemistry

Indian Institute of Technology Ropar, Rupnagar, Punjab, India.

Abstract:

Sulfur-derived functional groups can be found in a broad range of pharmaceuticals and natural products.¹ For centuries, sulfur has continued to maintain its status as the dominating heteroatom integrated into a set of 362 sulfur-containing FDA-approved drugs (besides oxygen or nitrogen) to the present. On the other hand, the chemistry of allenes has captivated globally due to its distinctive reactivity towards cycloaddition, cross-coupling, and cycloisomerization reactions.² However, there remains significant scope for further investigation into the diverse chemistry of allenes with variable substitution, such as sulfones. The presence of alcohol, sulfones, and allenes, designated as sulfonyl allenols, makes them structurally interesting³ and enhances their versatility, though this has not been extensively explored in organic transformations. The primary advantages of employing the sulfone group to activate an allene include its function as an electron-withdrawing group, which enhances reactivity, and it can be easily functionalized through various methods.³ Our research group is currently focused on using sulfonyl allenols to synthesize biologically significant compounds and fluorophores for medicinal chemistry, material science, and bioimaging, primarily employing metal catalysis.⁴

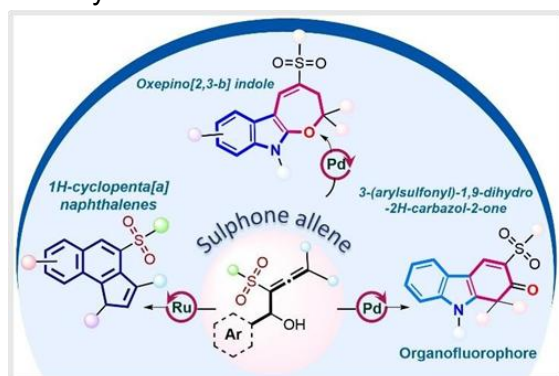


Figure 1: Reactivity of Sulfonyl allene

Reference:

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Bio-Sketch of the Speaker

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Research Career

Aslam has been an Assistant Professor at the Indian Institute of Technology Ropar (IIT RPR) since March 2023. He obtained an MSc (2012) in Chemistry and then pursued his PhD (2018) studies at CSIR-NCL, Pune, with a Prestigious Shyama Prasad Mukherjee Fellowship (SPMF), under the supervision of Dr Nitin T. Patil. In August 2018, he subsequently undertook PDRA positions at the University of California, Los Angeles, with Professor Ohyun Kwon, focusing on phosphine catalysis, and at the University of Arizona, Tucson, with Professor Thomas Gianetti, exploring Lewis acid catalysis and photocatalysis. Before joining IIT-Ropar as an Assistant Professor in the Department of Chemistry, he worked as a synthetic organic chemist at King Abdullah University of Science and Technology, Saudi Arabia, under the guidance of Professor Mohamed Eddaoudi.

Research Interest

Currently, Aslam's research group encompasses a broad spectrum of interests, emphasizing the development of methodologies for synthesizing biologically significant cores and fluorophores with relevance in medicinal chemistry, material science, and bioimaging. Metal catalysis serves as a central technique in their synthetic approaches. Additionally, they are exploring innovative low-energy photoredox processes to synthesize novel molecular architectures. Their work also extends into material chemistry, aiming to design compounds with optoelectronic properties and various related applications. Looking ahead, he plans to launch projects focused on electrophotochemistry to further expand the group's research horizons. His objective is to innovate sustainable approaches for drug development and to advance the use of organic fluorophores. He has also begun collaborating with researchers in the biomedical field to investigate the bioactivity of the compounds synthesized in his laboratory. Furthermore, his long-term aspiration involves partnering with AI research teams within the institute to create more efficient methodologies for synthesis processes.

Awards and Recognitions

Member of the Royal Society of Chemistry (MRSC), through RSC - Leader in the Field Nomination 2025
SERB-Startup Research Grant (SRG)- Electro-photocatalysis: Merging Light and Electricity to generate a sustainable way for Catalytic Organic Transformations 2023.

Aug 2021, Postdoctoral Professional Development Certificate by the University of Arizona.

Seal of Excellence awarded for Quality Proposal from MSCA-Horizon 2020 in March 2019.

Postdoctoral fellowship award at University of California Los Angeles 2018

Postdoctoral fellowship award at University of Arizona Tucson 2019

"RAJAPPA AWARD" - "Best Published Research Paper in Organic Chemistry" with the highest impact factor for the year 2017. Science Day Poster Session, CSIR-National Chemical Laboratory, Pune, February 2017 (Best Poster Prize), 21th ICOS International Symposium in Chemistry (ICOS-21), Indian Institute of Technology Bombay, December 2016.

"NCL-Agnimitra Memorial Best Poster Award" -Award best poster award on Feb-2017.

Science Day Poster Session, CSIR-National Chemical Laboratory, Pune, February 2015.-Best Poster award.

Publications in Journals & Patents

37 publications and 4 patents.

Details of projects handled- 2

OL3

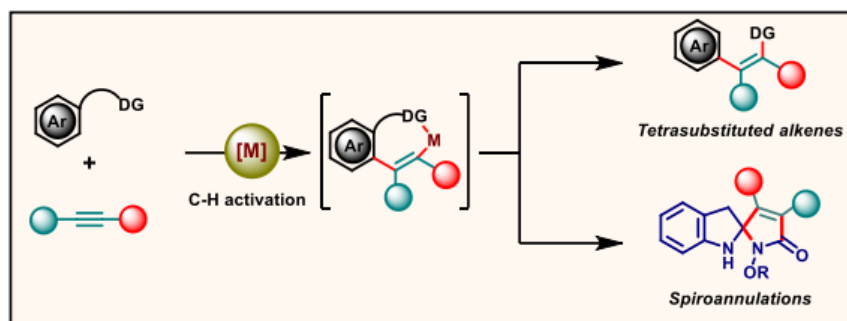
Three-Pronged Strategy: via Directing Group-Assisted Transition metal catalyzed Cascade Annulations

Dr. Vinaykumar Kanchupalli*

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Abstract: Transition metal-catalyzed, directing group (DG)-assisted selective C–H functionalizations and annulations represent a pivotal strategy in drug discovery and the synthesis of complex molecules.[1] However, achieving these transformations within the framework of traditional cross-coupling paradigms remains a formidable challenge. The directing group plays a crucial role in ensuring high site-selectivity and reactivity during these transformations. Notably, the termination steps of such reactions are influenced by the choice of directing groups and reaction conditions, leading to diverse outcomes. To address these challenges, various synthetic strategies have been developed, leveraging the complementary reactivities of DG-assisted approaches.

However, DG-assisted regioselective C–H functionalization followed by directing group (DG) migration remains an underexplored area.[2] Building on our group's interest in C–H functionalization strategies, this presentation will highlight our recent advancements in this emerging field. Specifically, I will discuss the synthesis of tetrasubstituted alkenes, spiro- γ -lactams, and related frameworks, showcasing their potential applications in complex molecule synthesis and medicinal chemistry. (**Scheme 1**).[3]



Scheme 1. Synthesis of tetrasubstituted alkenes and cascadeannulations via TM-catalyzed C-H Functionalizations

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- 3) a) Kumar, S.; Nunewar, S.; Usama, K. M.; **Kanchupalli, V.*** *Eur. J. Org. Chem.* **2021**, *2021*, 2223. b) Kumar, S.; **V. Kanchupalli*** *Org. Lett.* **2024**, *26*, 8975–8981.

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Dr. Vinay Kumar Kanchupalli was born and raised in Andhra Pradesh, in the southern part of India. He obtained his Bachelor of Science and Master of Science degrees in Organic Chemistry from Andhra University. He then pursued his doctoral studies under the supervision of Dr. Sreenivas Katukojvala at IISER Bhopal, where his research focused on the design and synthesis of diverse enalcarbenoids and their applications. Following his Ph.D., he carried out postdoctoral research at Loyola University Chicago and IIT Bombay.

In 2019, Dr. Kanchupalli began his independent research career at NIPER-Hyderabad as a DST Inspire Faculty, and later continued as a SERB Research Scientist. In 2024, he joined the School of Chemistry, University of Hyderabad, as an Assistant Professor. His current research focuses on the design and development of transition metal- and photocatalyzed synthetic transformations, with applications in the construction of natural products and biologically active molecular scaffolds.

Notable awards:

- M.Sc. (Organic Chemistry), Gold Medal for the Best Outgoing Student-2009.
- DST Inspire Faculty Award 2019-23.
- SERB Research Scientist (SERB-SRS) 2024-25.
- OPPI Young Scientist Award for the year-2023.
- Thieme Chemistry Journals Award-2025.

IL9

Engineering Earth-Abundant Metal Catalysts using Metal-Organic Frameworks for Selective Methane Functionalization

Kuntal Manna

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Abstract:

The direct oxidation of methane to valuable oxygenates, such as alcohols and acetic acid, is highly challenging under mild conditions due to high C–H bond dissociation energy, facile overoxidation to CO and CO₂ and the intricacy of C–H activation/C–C coupling. To address this challenge, we have developed multifunctional porous metal-organic frameworks (MOFs) catalysts using earth-abundant metals for direct methane oxidation into methanol or acetic acid selectively at different reaction conditions using O₂. The heterogeneous MOF-supported single-site copper(II) hydroxyl catalyst gives exceptionally high acetic acid productivity of 1,57,366 $\mu\text{mol}_{\text{CH}_3\text{CO}_2\text{H}} \text{g}_{\text{Cu}}^{-1} \text{h}^{-1}$ in 100% selectivity at 115 °C in water. Additionally, MOF nodes supported monomeric Fe^{III}(OH)₂ species yields methanol or acetic acid with high productivities of 38,592 $\mu\text{mol}_{\text{CH}_3\text{OH}} \text{g}_{\text{Fe}}^{-1} \text{h}^{-1}$ and 81,043 $\mu\text{mol}_{\text{CH}_3\text{CO}_2\text{H}} \text{g}_{\text{Fe}}^{-1} \text{h}^{-1}$, respectively. Through spectroscopic analyses, controlled experiments and computational studies, we demonstrate that the active-site isolation of mononuclear metal-hydroxyl species at the MOF nodes, their confinement within the porous framework, and their electron-deficient nature facilitate methane C–H activation via σ -bond metathesis, leading to the formation of liquid oxygenates in excellent selectivity. Our rational design of MOF-based base-metal catalysts and the reaction mechanism offers a sustainable route for methane valorization utilizing only O₂ and H₂O in a single-step, alternative to the capital-intensive syngas route. Additionally, we will discuss our recent advancements in abundant-metal catalyzed methane C–H borylation.

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Research Career

Ph. D. (Prof. Aaron D. Sadow), Iowa State University, Ames, USA, 2007-2012; Postdoctoral Research Scholar (Prof. Wenbin Lin), The University of Chicago, Chicago, IL, USA, 2013-2017; Assistant Professor, Indian Institute of Technology Delhi, Jan 2017- March 2022; Associate Professor, Indian Institute of Technology Delhi, April 2022 - present.

Research Interest

Organometallic chemistry, Porous functional materials, C-H bond activation, Heterogeneous catalysis

Awards and Recognitions

- The CRSI (Chemical Research Society of India) Bronze Medal
2026
- Humboldt Research Fellowship for Experienced Researchers, Germany
2025
- Emerging Investigators, Chemical Communications, RSC
2024
- Early Career: Mrs. Veena Arora Faculty Research Award, IIT Delhi
2022
- EurJIC Talents, Chemistry Europe
2022
- Emerging Investigators, Catalysis Science & Technology, RSC
2022
- Early Career Chemist Grant, Pacifichem, USA
2021
- Harvinder Singh Sawhney Young Faculty Incentive Fellowship, IIT Delhi
2017

IL10

Evolution of Co(III)-Catalysis in Asymmetric C-H Bond Functionalizations

Abir Das,¹ Harihara S. Ravishankar,¹ Subramani Kumaran,¹ **Basker Sundararaju***

¹ Department of chemistry, Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh, India -208016.

Abstract: Since Murahashi's groundbreaking work on cobalt-catalyzed C-H bond carbonylation in 1955,¹ the field of C-H bond functionalization has made significant strides, particularly with the development of low-valent cobalt systems.² While the use of in situ-generated or isolated cobalt(III) catalysts for C-H activation was seldom explored until the independent studies by Matsunaga and Daugulis in 2014,³ recent advancements have shed light on the intricate coordination environment around cobalt and the mechanisms driving these catalytic cycles.^{4e-f} In this talk, I will review the progress made over the past decade in Co(III)-catalyzed C-H bond functionalization,⁴⁻⁶ focusing on both mono- and bidentate directing groups, and the role of spectator ligands in the latter. I will also discuss how replacing these spectator ligands with external chiral ligands can induce chirality at the metal center through an enantiodetermining C-H activation step, and how these factors impact the efficiency and selectivity of asymmetric transformations.⁵ Additionally, I will highlight our systematic efforts to replace Mn(II) with photocatalysts^{4c,6a} or oxygen as sole oxidants,^{6b} thereby eliminating the need for stoichiometric metal oxidants in asymmetric C-H bond annulations using the Co/Salox catalytic system.

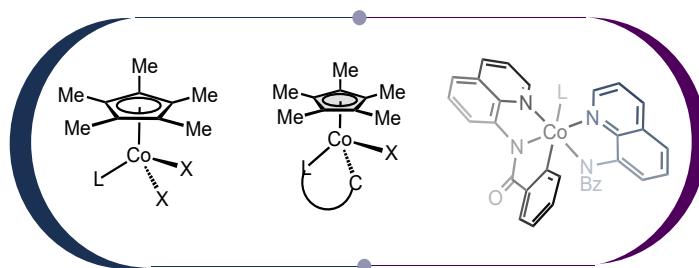


Figure 1: Overview Co(III) catalysts in C-H bond Functionalizations

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- [3] (a) L. Grigorjeva, O. Daugulis, *Angew. Chem. Int. Ed.* **53**, 10209-10212 (2014). (b) T. Yoshino, H. Ikemoto, S. Matsunaga and M. Kanai, *Angew. Chem. Int. Ed.* **52**, 2207-2211 (2013).
- [4] (a) M. Sen, B. Emayavaramban, N. Barsu, J. R. Premkumar, B. Sundararaju, *ACS Catal.* **6**, 2792-2796 (2016). (b) N. Barsu, S. K. Bolli, B. Sundararaju, *Chem. Sci.* **8**, 2431 (2017). (c) D. Kalsi, S. Dutta, N. Barsu, M. Rueping, B. Sundararaju, *ACS Catal.* **8**, 8115-8120 (2018). (d) N. Barsu, D. Kalsi, B. Sundararaju, *Catal. Sci. Technol.* **8**, 5963 (2018). (e) R. Mandal, B. Garai, B. Sundararaju, *ACS Catal.*, **12**, 3452 (2022). (f) R. Mandal, B. Garai, B. Sundararaju, *Science of Synthesis*, **3**, 149-260 (2023).
- [5] (a) B. Garai, A. Das, D. V. Kumar, B. Sundararaju, *Chem. Commun.* **60**, 3354 (2024). (b) A. Das, R. Mandal, H. S. Ravikumar, S. Kumaran, J. R. Premkumar, D. Borah, B. Sundararaju, *Angew. Chem. Int. Ed.* **63**, e202315005 (2024).
- [6] (a) V. Dwivedi, D. Kalsi, B. Sundararaju, *ChemCatChem*, **11**, 5160 (2019). (b) A. Das, S. Kumaran, H. S. Ravi Shankar, J. R. Premkumar, B. Sundararaju, *Angew. Chem. Int. Ed.*, **63**, e202406195 (2024). (c) A. Das, S. Kumaran, P. Maity, J. Richard Premkumar, B. Sundararaju, *J. Am. Chem. Soc.* **147**, 26226 (2025). (d) S. Kumaran, A. Das, J. Richard Premkumar, B. Sundararaju [Chemrxiv](https://doi.org/10.26434/chemrxiv-2025-8bk3h), DOI: 10.26434/chemrxiv-2025-8bk3h (2025).

Bio-Sketch of the Speaker

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Kanpur, Uttar Pradesh, India – 208016.

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E-mail: basker@iitk.ac.in



Research Career

Since 2022 Professor, Department of chemistry, IIT Kanpur, Kanpur, India

2018-2022 Associate Professor, Department of chemistry, IIT Kanpur, Kanpur, India

2014-2018 Assistant Professor, Department of chemistry, IIT Kanpur, Kanpur, India

2013-2018 Assistant Professor (cont), Department of chemistry, IIT Kanpur, Kanpur, India

2011-2013 Postdoctoral Fellow at Max-Planck Institute of Coal Research, Muelheim (with Prof. Alois Fuerstner)

2008-2011 PhD, Université de Rennes1, Rennes, France

2008 MS, Université de Rennes1, Rennes, France

Research Interest

Catalysis driven Organometallic chemistry

3d Metal Asymmetric catalysis

C-H bond Functionalization, Hydrogenation, Asymmetric Photocatalysis

Awards and Recognitions

Merck Young Scientist Award 2019

Fellow of Royal Society of Chemistry 2022

Bronze Medal, Chemical Research Society of India 2023

Invited Guest professor at LCC-Université de Toulouse III – Paul Sabatier (Oct-Nov) 2024

Associate Fellow of Indian National Science Academy (IAF) 2025

Publications in Journals & Patents

89 publications, H-Index: 41, >5400 citations

Representative Publications

[1] A. Das, S. Kumaran, P. Maity, J. Richard Premkumar, B. Sundararaju, J. Am. Chem. Soc. 147, 26226 (2025).

[2] B. Garai, A. Das, D. V. Kumar, B. Sundararaju, Chem. Commun. 60, 3354 (2024). A. Das, R. Mandal, H. S. Ravikumar, S. Kumaran, J. R. Premkumar, D. Borah, B. Sundararaju, Angew. Chem. Int. Ed. 63, e202315005 (2024).

[3] A. Das, S. Kumaran, H. S. Ravi Shankar, J. R. Premkumar, B. Sundararaju, B. Angew. Chem. Int. Ed., 63, e202406195 (2024).

[4] M. Sen, B. Emayavaramban, N. Barsu, J. R. Premkumar, B. Sundararaju, ACS Catal. 6, 2792-2796 (2016).

[5] N. Barsu, S. K. Bolli, B. Sundararaju, Chem. Sci. 8, 2431 (2017).

[6] D. Kalsi, S. Dutta, N. Barsu, M. Rueping, B. Sundararaju, ACS Catal. 8, 8115-8120 (2018).

[7] R. Mandal, B. Garai, B. Sundararaju, ACS Catal., 12, 3452 (2022).

[8] R. Mandal, B. Garai, B. Sundararaju, Science of Synthesis, 3, 149-260 (2023).

IL11

N-Capped Short Peptide-conjugates for Therapeutic Applications

Amitava Das

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Abstract:

A key goal in modern therapeutic design is achieving spatiotemporal precision in delivering active agents to maximise efficacy while minimising systemic toxicity. This requires integrating molecular precision with biological complexity. Molecular recognition and stimuli-responsiveness offer promising routes for selective activation at disease sites. Advances in molecular recognition-based syntheses now enable finely tuned delivery systems with improved therapeutic indices and fewer off-target effects. Building on this foundation, we employ a scaffold-driven strategy using short, purpose-built peptides as modular platforms. Through proof-of-concept studies, we show how rationally engineered prodrugs and molecular composites can sense and respond to biological cues, advancing the design of next-generation precision therapeutics.

References:

- 1) Dutta, S.; Tripathy, S.; Bej, S.; Parvin, S.; Jana, B.; Patra, C.R.; Das, A.; Chem. Sci. (2025) 16, 16573 - 16583; N; Kandoth, N; Gupta, S.; Raksha, K.; Gupta, S.; Chaudhary, S.P.; Pramanik, S.K.; Mallick, A.I.; Bhattacharyya, S.; Das, A. Adv. Funct. Mater. (2024) 240099; Pramanik, S. K., Sreedharan, S., Kandoth, N.; Das, A.; Thomas, J. A. Nature Chem. Rev. (2025) <http://doi.org/10.1038/s41570-025-00764-w>.
- 2) Sarkar, S.; Atin Chatterjee, A.; Kim, D.; Saritha, C.; Barman, S.; Jana, B.; Ryu, J-H.; Das, A. Adv Healthc Mater. (2025) 24, 2403243; Bose, S.; Sen, S.; Mariam, T.; Jana, A.; Pal, U.; Jana, B.; Ghosh, S.; Das, A. J. Am. Chem. Soc. (2025) <https://doi.org/10.1021/jacs.5c11249>.
- 3) Chatterjee, A.; Sarkar, S.; Bhattacharjee, S.; Bhattacharyya, A.; Barman, S.; Pal, U.; Pandey, R. Ethirajan, A.; Jana, B.; Das, B.B.; Das, A. J. Am. Chem. Soc. (2025) 147, 532–547.

Bio-Sketch of the Speaker

Dr. Amitava Das.

Professor

Dept: Chemical Sciences (DCS)

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Indian Institute of Science Education and Research Kolkata.

Research Interest:

Molecular Recognition; Supramolecular Chemistry; Stimuli-responsive nanostructured material, Stimuli-responsive drug release and Imaging Reagents.

Research Career:

Academic Background:

- Ph.D. (Inorganic Reaction Mechanism), Jadavpur University, 1989
- M.Sc. (Analytical Chemistry), Jadavpur University, 1985
- B.Sc. (Chemistry), Jadavpur University, 1983

Positions:

- Professor, IISER Kolkata (current)
- Director, CSIR-Central Salt & Marine Chemicals Research Institute (2016 - 2019)
- Chief Scientist, CSIR-National Chemical Laboratory (2013 - 2016)
- Scientist, CSIR-Central Salt & Marine Chemicals Research Institute (1992 - 2013)
- Post-doctoral Fellow, University of Bristol (1990 - 1992)
- Post-doctoral Fellow [Nehru Fellowship], University of Birmingham (1989 - 1990)
- Research Fellow, Jadavpur University (1986 - 1989)
- Process Executive, Dytron India Ltd. (1985 - 1986)
-

Awards and Honors:

- *Prof. P. K. Bhattacharya Gold Medal Lecture Series Award* from M.S. University, Vadodara (2020)
- *SERB-J.C. Bose National Fellow-Second Term Since April 2023* from DST-SERB (2017)
- *Fellow of Indian National Science Academy* from Indian National Science Academy (2017)
- *CRSI Silver Medal* from Chemical Research Society of India (2016)
- *Fellow of Gujarat Science Academy* from Gujarat Science Academy (2016)
- *Prof. Suresh C. Ameta award of Indian Chemical Society* from Indian Chemical Society (2015)
- *Fellow of Royal Society of Chemistry* from Royal Society (2014)
- *Fellow of the National Academy of Science* from National Academy of Science (2012)
- *Fellow of the Indian Academy of Science* from Indian Academy of Science (2010)
- *CRSI Bronze Medal* from Chemical Research Society of India (2009)

Day1 – 17-11-2025, Auditorium 2

IL6

Taming Radicals: Strategies for Bond Activation and Functionalization

Bhisma Kumar Patel¹ Department of Chemistry, Indian Institute of Technology, IIT Guwahati-781039, INDIA.

Abstract: Radical-mediated reactions enable unique bond-forming pathways that are often inaccessible through traditional ionic or concerted mechanisms. Our research group has been generating N-, S-, and C-centered radicals via thermal, photochemical, and electrochemical methods, leading to a variety of novel and synthetically valuable organic transformations. The N-centred radicals (NCRs) have emerged as powerful intermediates for constructing diverse nitrogen-containing heterocycles under mild and sustainable conditions. *tert*-Butyl nitrite (TBN) has proven to be a versatile precursor, functioning as both N and N–O synthon, enabling efficient C–N and N–O bond formations in the synthesis of nitrogenous heterocycles.^[1] An intermolecular radical-based distal selectivity in appended alkyl chains has been developed. The selectivity is maximum when the distal carbon is γ to the appended group and decreases by moving from $\gamma \rightarrow \delta \rightarrow \epsilon$ positions.^[2] The thiol radical generated under photochemical conditions, either from the thiol of the disulfide, can trigger a reaction leading to *the bis-functionalization of maleimide or cascade cyclisation*, forming thiofunctionalized pyrrole or pyridine.^[3] The EDA (Electron Donor–Acceptor) complex–based photochemical synthesis is important in modern organic chemistry as it absorbs visible light directly, often without **photocatalysts, leading to useful C–C, C–N, C–S, and C–O bond-forming transformations.**^[4] Further demonstrated is an external photo-sensitizer-free (auto-sensitized) singlet oxygen-enabled solvent-dependent tertiary hydroxylation and aryl-alkyl spirocyclic etherification of C3-maleimidated quinoxalines. Such photochemical “reagent-less” oxygenation at $sp^3C\text{---}H$ and etherification involving $sp^3C\text{---}H$ and $sp^2C\text{---}H$ are unparalleled.^[5] An operationally simple EnT-mediated C3-*N*-heteroarylation of 2-aryl quinoxalines *via* decarboxylative radical-radical cross-coupling ($Csp^2\text{---}Csp^2$) with oxime esters is accomplished.^[6] Mechanistic studies supported by DFT calculations reveal that spin density distribution and thermodynamic stability dictate regioselectivity in some of these transformations.

References:

- [1]. (a) Sau, P.; Santra, S. K.; Rakshit, A.; Patel, B. K. *J. Org. Chem.* **2017**, *82*, 6358. (b) Sau, P.; Rakshit, A.; Modi, A.; Behera, A.; Patel, B. K. *J. Org. Chem.* **2018**, *83*, 1056. (c) Sau, P.; Rakshit, A.; Alam, T.; Srivastava, H. K.; Patel, B. K. *Org. Lett.* **2019**, *21*, 4966. (d) Alam, T.; Rakshit, A.; Begum, P.; Dahiya, A.; Patel, B. K. *Org. Lett.* **2020**, *22*, 3728. (e) Rajamanickam, S.; Sah, C.; Mir, B. A.; Ghosh, A.; Sethi, G.; Yadav, V.; Venkataramani, S.; Patel, B. K. *J. Org. Chem.* **2020**, *85*, 2118.
- [2]. Rajamanickam, S.; Saraswat, M.; Venkataramani, S.; Patel, B. K. *Chem. Sci.* **2021**, *12*, 15318.
- [3]. (a) Khanddelia, T.; Ghosh, S.; Patel, B. K. *Chem. Commun.* **2023**, *59*, 2118. (b) Sahoo, A. K.; Rakshit, A.; Dahiya, A.; Pan, A.; Patel, B. K. *Org. Lett.* **2022**, *24*, 1918. (c) A K Sahoo, A Rakshit, A Pan, H N Dhara, and B K Patel,* *Org. Biomol. Chem.* **2023**, *21*, 1680.
- [4]. Barik, D.; Chakraborty, N.; Sahoo, A. K.; Dhara, H. N. Patel, B. K. *Chem. Commun.*, **2024**, *60*, 12577. (b) Dhara, H. N.; Rakshit, A.; Barik, D.; Ghosh, K. Patel, B. K. *Chem. Commun.*, **2023**, *59*, 7990.
- [5]. Ghosh, S.; Khandelia, T.; Mahadevan, A.; Panigrahi, P.; Kumar, P.; Mandal, R.; Boruah, D.; Venkataramani, Patel, B. K. *Chem Eur. J.*, **2024**, e202400219.
- [6]. Mandal, R.; Ghosh, S.; Laha, S.; Panigrahi, P.; Bhattacharyya, K.; Patel, B. K. *Org. Lett.*, **2025**, *27*, 4257

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Prof. Bhisma K Patel

Department of Chemistry
Indian Institute of Technology Guwahati
North Guwahati-781039
Assam, India
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Research Career

- Ph. D. (1994) Chemistry, Indian Institute of Technology Kanpur.
- Post-Doc (1994-1997), Max-Planck Institute for Exp. Medicine, Gottingen, Germany

Research Interest

Catalytic organic processes, involving metal-, electro-, and photocatalysis.

Awards and Recognitions

- Members of the Editorial Board of Tetrahedron and Tetrahedron Letters (2024)
- Prof. G. B. V Subramanian Memorial Lecture, University of Delhi (2024).
- Associate Editor, Journal of Chemical Sciences (Since 2022)
- Prof. D. S. Bhakuni Award, by the Indian Chemical Society (2018).
- Prof. M. K. Rout memorial lecture by Odisha Chemical Society (2018).
- Fellow of the Indian Academy of Sciences, (FASc), 2017.
- Fellow of the National Academy of Science (NASI) (FNASc), India 2017.
- Recipient Coastal Chemical Research Society Award (CCRS-2016)
- Recipient of Samanta Chandra Sekhar Award by Odisha Bigyan Academy 2015.
- Awarded Bronze Medal by Chemical Research Society (CRSI) of India 2014.
- R. C. Tripathy Young Scientist Award by Orissa Chemical Society (OCS) 1998.

Publications in Journals & Patents

Scientific publications-212, Book Chapters-19, Patent 02

Details of projects handled

15

IL7

Catalytic Synthesis of Chiral Swaminathan Ketones and Miltirones

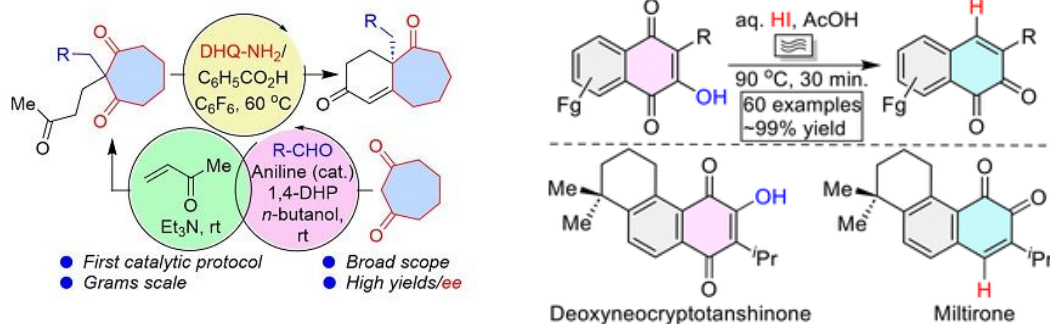
Dhevalapally B. Ramachary*

Catalysis Laboratory, School of Chemistry, University of Hyderabad,
Central University P.O., C. R. Rao Road, Gachibowli, Hyderabad 500 046, Telangana, INDIA
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Abstract:

Recently, we developed an unprecedented, metal-free, three-step, sustainable catalytic asymmetric desymmetrization of conformationally flexible 2-alkyl-2-(3-oxobutyl)-cycloheptane-1,3-diones to produce library of chiral Swaminathan ketones, which are part of many natural products and drugs.¹ The most crucial and essential ongoing global research is to convert the abundantly available feedstock into materially and medicinally valuable scaffolds in a greener mode. This requires the proper selection of feedstock and the development of systematic green synthetic strategies to convert it into valuable entities. One of the most attractive and abundant feedstocks is lawsones. However, the selective removal of the enolic hydroxy group from the dynamic tautomers of lawsones to access 1,2- and/or 1,4-naphthoquinones, which have plenty of synthetic applications, remains a challenge. Recently, we reported metal-free, chemo-/regio-selective high-yielding hydrodehydroxylation (HDH) strategies in which the abundantly available 3-alkylawsones were treated with aqueous HI in AcOH under microwave irradiation for a few minutes to access a vast library of materially and medicinally important 1,2-naphthoquinones. We also reported the short total synthesis of medicinally important drug molecules, such as deoxyneocryptotanshinone, miltirone, and vitamin-K3 (menadione) and their analogues, using the currently developed HDH as a key reaction.²

In this lecture will discuss saga of these reaction's development.

**References:**

- [1] A. V. Krishna, S. D. Sanwal, S. Rath, P. R. Lakshmi, D. B. Ramachary, *Green Chem.* **2024**, 26, 771-784.
- [2] S. Rath, P. Lamba, P. S. K. Reddy, A. V. Krishna, D. B. Ramachary, *Green Chem.* **2025**, 27, 3465-3476.

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Homepage: <http://chemistry.uohyd.ac.in/~icccs8/index.html>



Research Career

Ramachary graduated with M.Sc. degree in School of Chemistry from University of Hyderabad and obtained Ph.D. in synthetic organic chemistry from the Indian Institute of Science, Bangalore in 2001. He subsequently held postdoctoral position at the Scripps Research Institute for Catalysis in 2002-2005, prior to joining University of Hyderabad in January 2005, where presently he is senior professor of organic chemistry.

Research Interest

Synthetic Organic Chemistry (Both Total Synthesis and Reaction Engineering)
Asymmetric Supramolecular Catalysis and Organocatalysis
Development of Multi-Component and Multi-Catalysis Cascade Reactions
Application of Organocatalysis in Other Disciplines

Awards and Recognitions

Fellow of the all Three Academies of India

Publications in Journals & Patents

125

Details of projects handled

10

Technology development/ Initiation

- 1) Organocatalytic Reductive Coupling Reaction for C-C Bond Formation,
- 2) Organocatalytic [3+2]-Cycloaddition for Click Reaction,
- 3) Organocatalytic Aminoalkyne-catalysis,
- 4) Base Induced Ring Opening (BIRO) Reaction for Z-Dienes,
- 5) Organocatalytic Azide-Carbonyl [3+2]-Cycloaddition for 1,2,3-Triazoles.

Others

He is a recipient of many awards including Fellow of the National Academy of Sciences, Allahabad-2021, Fellow of the Royal Society of Chemistry, London-2020 and Fellow of Indian Academy of Sciences, Bangalore-2018. He has guided 22-PhD students, 14 PDFs and out of them, 5-PhD's got Eli Lilly & Company Asia Outstanding Thesis Awards 2011, 2012, 2013, 2014 and 2021. He is an Editorial Advisory Board Member, Organic & Biomolecular Chemistry, RSC Journal 2013-present; Editorial Advisory Board Member, European Journal of Organic Chemistry, Wiley Journal 2017-present; Editorial Advisory Board Member, Tetrahedron Chem, Elsevier Journal 2021-present; Editorial Advisory Board Member, Tetrahedron/Tetrahedron Letters, Elsevier Journals 2024-present; and Editorial Advisory Board Member, Sustainability and Circularity NOW, March 2025 to Present. Prof. Ramachary serving as a reviewer for many national and international reputed journals and member in many committees of national funding body, DST, SERB. Prof. Ramachary published more than 125 research papers in both national and international reputed journals, two books on emerging organocatalysis area and few chemical reactions are named after him.

IL8

π -Conjugated Molecular Assemblies with Dynamic Functions across Nano- to Macro-Scales

Atsuro TAKAI^{1,2*}

¹ National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, Ibaraki, Japan.

² University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki, Japan

Abstract:

π -Conjugated molecules are fundamental components for organic optical and electronic materials. In addition to their excellent physicochemical properties, we have been developing π -conjugated molecules and their supramolecular assemblies endowed with novel dynamic functions such as stimuli-responsiveness and autonomous behavior. To realize these functions, we have pursued original molecular designs and developed click reactions—including a catalyst-free click reaction between electron-accepting π -conjugated molecules and amines.^[1,2] In this presentation, we introduce π -systems exhibiting dynamic properties across scales from the nano- to the macro- scales (**Figure 1**).^[3,4]

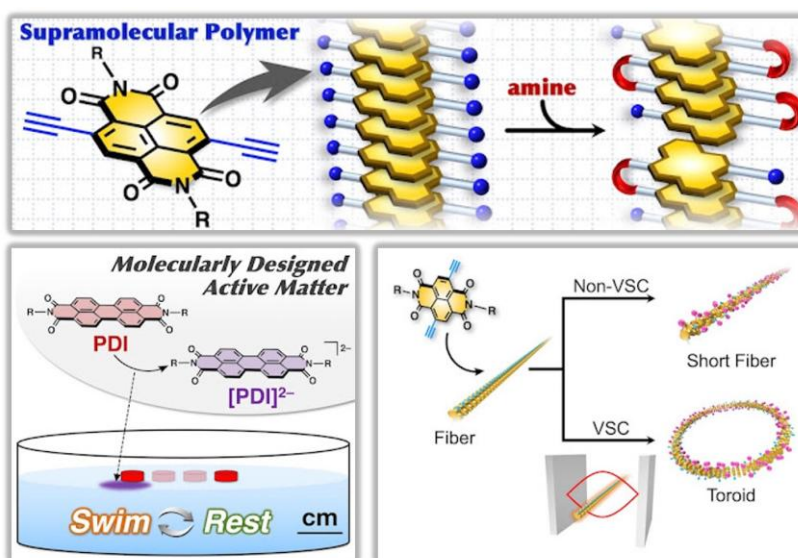


Figure 1 Overview of this presentation on stimuli responsive, dynamic π -conjugated molecular assemblies.

References:

- [1] M. Tan, M. Takeuchi, A. Takai* *Chem. Sci.* 13, 4413 (2022).
- [2] S. Imai, T. Hamada, M. Nozaki, T. Fujita, M. Takahashi, Y. Fujita, K. Harano, H. Uji-i, A. Takai*, K. Hirai* *J. Am. Chem. Soc.* 147, 23528 (2025).
- [3] L. R. Holstein, N. J. Suematsu, M. Takeuchi, K. Harano, T. Banno, A. Takai* *Angew. Chem. Int. Ed.* 63, e202410671 (2024).
- [4] L. R. Holstein, M. Takeuchi, N. J. Suematsu, A. Takai* *J. Am. Chem. Soc.* 147, 40024 (2025).

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Research Career

He was educated at Osaka University, Japan. He received his Ph.D. (2011) from Osaka University under the direction of Professor Shunichi Fukuzumi. During his Ph.D. studies, he collaborated with professors Roger Guillard and Jean-Michel Barbe at Université de Bourgogne, France.

He later became a JSPS (Japan Society for the Promotion of Science) postdoctoral researcher at the Organic Materials Group, National Institute for Materials Science (NIMS), Japan, working with Professor Masayuki Takeuchi. From March 2013 to August 2014, he worked for Professors Antonio Facchetti and Tobin J. Marks at Northwestern University, USA. After spending a few years as a tenure-track researcher at the International Center for Young Scientists (ICYS) at NIMS, he was appointed as a tenured senior researcher. He is also an Associate Professor at University of Tsukuba.

Research Interest

Organic Materials Chemistry, Supramolecular Chemistry, Electron-Transfer Chemistry

Awards and Recognitions

102nd CSJ (The Chemical Society of Japan) Young Scholar Lecture, 2022.3

95th CSJ (The Chemical Society of Japan) Presentation Award, 2015.3

Publications in Journals & Patents

40 Peer Reviewed International Journals

6 Review Articles and Book Chapter (in Japanese)

1 U.S. Patent

Details of projects handled

13

SL5

CuH-Catalyzed Enantioselective Alkoxyallylation

Rambabu Chegondi*

Organic Synthesis and Process Chemistry Department

CSIR-Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad 500007, India

Email: rchegondi@iict.res.in**Abstract:**

Enantiomerically enriched complex alcohols are presented in wide range of small molecule therapeutics and biologically active natural polyketides. Therefore, exploring the general methods for the enantioselective synthesis of substituted alcohols is an attractive target in organic synthesis.^[1,2] Here, we have developed the Cu(I)-catalyzed enantioselective hydrocupration¹⁻² for the synthesis of complex 1,2-*syn-sec,tert*-diols, α -hydroxy allyl ketones and propargyl alcohols using reductive coupling of carbon-carbon π -bonds with carbonyl compounds.^[3,4]

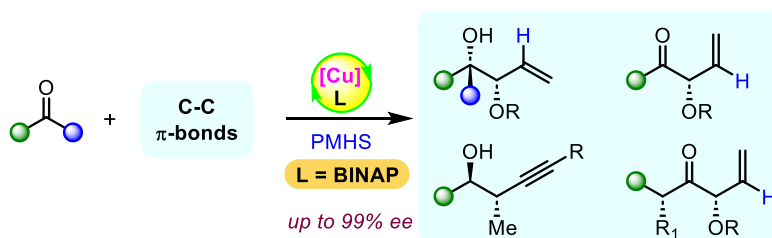


Figure. Enantioselective hydrocupration to access chiral alcohols

References and notes:

1. S. B. Jadhav, S. R. Dash, S. Maurya, J. B. Nanubolu, K. Vanka, R. Chegondi, *Nat. Commun.* **2022**, *13*, 854.
2. V. B. Patil, S. B. Jadhav, J. B. Nanubolu, R. Chegondi, *Org. Lett.* **2022**, *24*, 8233.
3. Navaneetha, N.; Maurya, S.; Behera, P.; Jadhav, S. B.; Magham, L. R.; Nanubolu, J. B.; Roy, L.; Chegondi, R. *Chem. Sci.* **2024**, *15*, 20379.
4. Maurya, S.; Navaneetha, N.; Behera, P.; Nanubolu, J. B.; Roy, L.; Chegondi, R. *Angew. Chem. Int. Ed.* **2025**, e202420106.

Bio-Sketch of the Speaker

Dr. Rambabu Chegondi

Senior Principal Scientist

Department of Organic Synthesis & Process Chemistry

CSIR-Indian Institute of Chemical Technology (CSIR-IICT)

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Homepage: <https://cramhcu.wixsite.com/rambabu-chegondi>



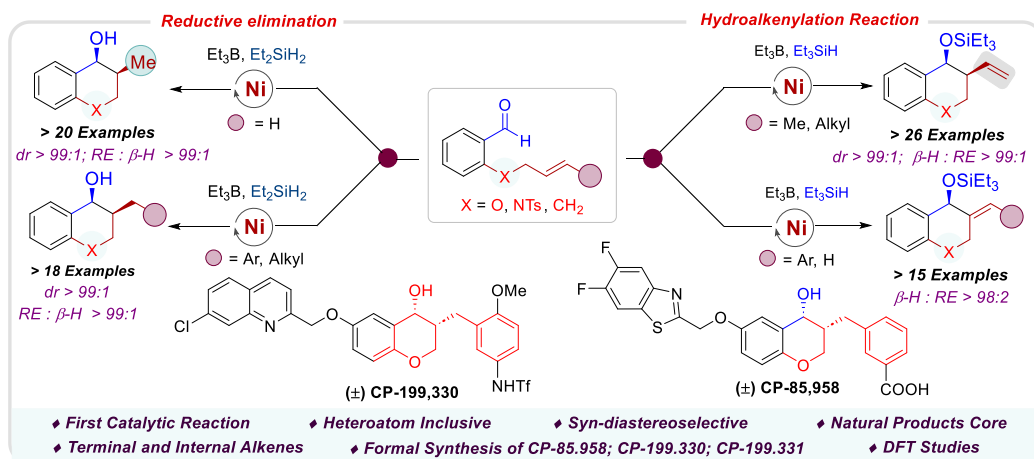
Rambabu Chegondi received his M.Sc. (2003) from the University of Hyderabad and completed his Ph.D. (2009) in Organic Synthesis at the CSIR-Indian Institute of Chemical Technology (IICT), Hyderabad, under the supervision of Dr. S. Chandrasekhar. In 2009, he moved to the University of Kansas, USA, where he worked as a postdoctoral researcher with Prof. Paul R. Hanson. He returned to CSIR-IICT in 2014 as a CSIR-Pool Scientist (SRA), beginning his independent research career. He is currently a Principal Scientist in the OS&PC Department at CSIR-IICT, focusing on the development of new enantioselective desymmetrization methodologies and process development of key APIs.

Dr. Chegondi's contributions have been recognized with several honors, including the Eli Lilly Asia Best Thesis Award (2009), AVRA Young Scientist Award (2019), Thieme Chemistry Journals Award, SERB-STAR Award, and the CRSI Bronze Medal (2026). He is a Fellow of the Royal Society of Chemistry (FRSC) and serves on the Editorial Advisory Board of Organic Letters.

SL6

Nickel(0)-Catalyzed Oxidative Cyclization of π -SystemsVenkataraman Ganesh^{1*}, Sudipta Ghosh², Rajesh Chakraborty³¹ Department of Chemistry, Indian Institute of Technology Kharagpur, West Bengal – 721302, India**Abstract:**

Nickel(0) complexes have been traditionally stored and used under highly controlled environments. Our research focuses on bringing sensitive nickel chemistry to the benchtop. Here, we present our recent work on Ni(0)-catalyzed alkene-aldehyde coupling to access *syn*-chromanols. *Syn*-chromanol motifs are prominent in various bioactive natural products, pharmaceuticals, and drug molecules.¹ We demonstrate a nickel(0)-catalyzed intramolecular reductive coupling of *O*-allylsalicylaldehyde to afford a chromanol compound with exclusive *syn* selectivity.² We have successfully addressed two major challenges of this reaction: (a) Tsuji-Trost type deallylation of *o*-homoallyloxy benzaldehyde to give salicylaldehyde back, (b) competing hydrosilylation of aldehyde moiety in the presence of silane. This methodology is applicable to both terminal and internal alkenes. The choice of reducing agent is crucial for controlling the reactivity of the 5-membered nickelacycle intermediate towards a reductive elimination or a β -hydride elimination pathway. Using this methodology, the formal synthesis of drug molecules, such as CP-85,958 and CP-199,330, has been demonstrated. Along similar lines, a regioselective [2 + 2 + 2] cyclotrimerization of 1,3-diynes catalyzed by Ni(0) has been demonstrated to provide hexasubstituted benzenes (HSBs). The present protocol exhibited remarkable versatility, transforming 1,3-diynes with diverse alkyl, aryl, and heterocyclic groups to the corresponding HSBs. With the aid of control experiments and density functional theory (DFT), the reaction mechanism and the origin of regioselectivity were elucidated.

**References:**

- [1] Li, W.; Yang, T.; Song, N.; Li, R.; Long, J.; He, L.; Zhang, X.; Lv, H.; *Chem. Sci.*, **2022**, 13, 1808-1814.
- [2] Ghosh, S.; Rooj, A.; Chakraborty, R.; Ganesh, V.; *Org. Lett.* **2024**, 26, 4024-4029.
- [3] Ghosh, S.; Khamrai, A.; Ganesh, V.; *Org. Lett.* **2025**, ASAP (DOI: 10.1021/acs.orglett.5c03947)

Bio-Sketch of the Speaker

Dr. Ganesh Venkataraman

Department of Chemistry
IIT Kharagpur, West Bengal,
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Research Career

Venkataraman Ganesh received his early education from Bishop Heber College, Tiruchirappalli (2001-2004), and joined the Integrated Ph.D. program (Chemical Sciences) at the Indian Institute of Science (IISc), Bangalore (2004). Ganesh obtained his Ph.D. in 2013, working with Prof. S. Chandrasekaran as a CSIR-Shyama Prasad Mukherjee (CSIR-SPM) fellow. He had postdoctoral stints as a JSPS fellow (2013–15) with Prof. M. Shibasaki at BIKAKEN, Japan, and as a Newton International Fellow (2016–18) with Prof. V. K. Aggarwal at the University of Bristol, UK. He began his independent research career in 2018 at the Department of Chemistry, Indian Institute of Technology Kharagpur, India, and held the Ramanujan Fellowship until 2023 (SERB, India). His research interests include the exploitation of transition-metal catalysts and boron chemistry to develop new synthetic methodologies and conduct mechanistic studies.

Research Interest

Transition-metal catalysis; Boron chemistry; Synthetic methodologies and Mechanistic studies

Awards and Recognitions

Ramanujan Fellowship - SERB, Department of Science and Technology (2018-2023)
Newton International Fellowship – The Royal Society, London, UK (2016-18)
JSPS Postdoctoral Research Fellowship – Japanese Science and Technology (2013-15)
Shyama Prasad Mukherjee Fellowship – CSIR-SPM (2008-12)

Publications in Journals & Patents

Publications: 41
Patents (filled): 2

Details of projects handled

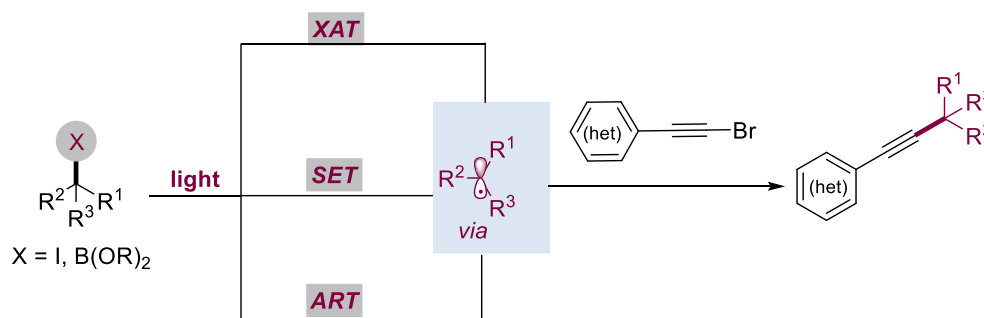
Extramural Grants: 4
IIT KGP Startup Grant: 1

SL7

Synthesis of Internal Alkynes via SET, XAT and ART

Veera Reddy Yatham¹¹School of Chemistry, Indian Institute of Science Education and Research, Thiruvananthapuram 695551, India.**Abstract:**

Alkynes are important and versatile building blocks in organic chemistry frequently appearing in natural products, bioactive compounds. The internal alkyne moiety allows numerous modifications for the synthesis of pharmacophores, fine chemicals and agrochemicals. Therefore, the construction of internal alkynes using a variety of alkyl radical precursors such as alkyl carboxylic acids and its derivatives, 4-alkyl-substituted Hantzsch esters (HEs), alkyl NHP esters, alkyl Katritzky salts, alkyl thianthrenium salts, alkyl iodides, alkyl-BF₃k, alkyl-Bpin and using excess of hydrocarbons have been reported using acetylenic sulfone or ethynylbenziodoxolone (EBX) as an alkynylating reagent. However, most of the developed methods produce large amounts of by-products that are generated either from alkyl radical precursor or alkynylating agent. Also, halo alkynes are important and widely used intermediates in synthetic chemistry. It has also been shown that these haloalkynes serve as effective alkynylating agents, thanks to their atom economy and ease of availability. In the present lecture I will discuss photoinduced synthesis of Internal alkynes via the concept of Halogen atom transfer (XAT), Single electron transfer (SET) and Amino radical transfer (ART).²

**Scheme 1.** Photoinduced synthesis of internal alkynes**References:**

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

Bio-Sketch of the Speaker

Dr. Veera Reddy Yatham,

Associate professor,
School of Chemistry
Indian Institute of Science Education and Research
Thiruvananthapuram (IISER TVM)
Maruthamala PO, Vithura, Kerala 695551,
India.



Professional Experience:

| | |
|---------------------------|--|
| 06 Feb 2025 – present | Associate Professor, IISER-TVM, India. |
| 31 Jan 2020 – 05 Feb 2025 | Assistant Professor, IISER-TVM, India. |
| 31 May 2019 – 27 Jan 2020 | Ramanujan fellow at CSIR-IICT, HYD, India. |

Research Experience:

| | |
|-----------------------|---|
| Aug 2018 – May 2019 | Post.doc with Prof. Bukhard konig , Department of chemie and Pharmazie University of Regensburg. |
| May 2016 – April 2018 | Post.doc with Prof. Ruben Martin Institute of Chemical Research of Catalonia (ICIQ), Spain. |

Academic qualifications:

| | |
|----------------------|--|
| Nov 2011 – June 2015 | Ph.D. with Prof. Albrecht Berkessel , Institute of Organic Chemistry, <i>University of Cologne, Germany</i> . |
| August 2008 - 2011 | Master of Science (MS) FROM <i>Indian Institute of Science (IISc), Bangalore, India</i> . |

SL8

Light-/Electricity-/Organocatalysis-Driven Divergent Stereoselective Reactions

Pankaj Chauhan*

Department of Chemistry, Indian Institute of Technology Jammu, J&K, India

Abstract:

The application of sustainable energy inputs and modern catalysis is transforming the way complex molecules are constructed. Harnessing visible light, electricity, or organocatalysis in organic synthesis provides unique opportunities to access structurally diverse and stereochemically rich scaffolds, often through divergent pathways originating from common starting materials. These strategies not only reduce dependence on precious metals but also enable precise control over chemo-, regio-, and stereoselectivity under mild and environmentally benign conditions. By leveraging the complementary features of these activation modes, it becomes possible to direct the same substrate into distinct product classes simply by altering the source of activation or the catalytic environment. In this context, the examples from our laboratory include the stereoselective divergent desymmetrization of cyclohexadienones,^[1] reactivities of styryl diazo compounds,^[2] and the stereoselective construction of bridged biaryls.^[3] In each case, divergence arises from the ability of different energy inputs to unlock unique reactivity patterns, which are then harnessed and controlled through carefully designed substrates. By expanding the boundaries of what can be achieved with light, electricity, and organocatalysis, these strategies open new avenues for innovation in stereoselective synthesis. In this talk, our recent efforts toward developing divergent stereoselective reactions assisted by light, electricity, and organocatalysis will be presented.

References:

- [1] a) D. Sharma, P. Sharma, V. Sodhi, M. Sharma and **P. Chauhan**, *unpublished results*. b) M. Sharma, V. Sodhi, Y. Hussain, D. Sharma, C. Empel and **P. Chauhan**, *unpublished results*. c) M. Sharma, and **P. Chauhan**, *Chem. Commun.* **2025**, 61, 1455-1458. d) V. Sodhi, D. Sharma, M. Sharma and **P. Chauhan**, *Org. Chem. Front.* **2025**, 12, 1144-1149. e) M. Sharma, Tamanna and **P. Chauhan**, *Org. Lett.* **2023**, 25, 7911-7916.
- [2] a) J. Kumar, D. Sharma, Y. Hussain, Solaim, J. Sinhmar, Muskan, A. Changotra and **P. Chauhan**, *Org. Lett.* **2025**, 27, 1608-1613. b) Y. Hussain, R. Prasanna, C. Empel, D. Sharma, L. Kloene, W. F. Zhu, A. Kaiser, L. Weizel, E. Proschak, R. M. Koenigs and **P. Chauhan**, *Angew. Chem. Int. Ed.* **2025**, 64, e202416956. c) Y. Hussain, C. Empel, R. M. Koenigs, **P. Chauhan**, *Angew. Chem. Int. Ed.* **2023**, 62, e202309184.
- [3] a) N. Kotwal, Solaim, D. Sharma, **P. Chauhan***, *unpublished results*. b) N. Kotwal, Tamanna, A. Changotra, **P. Chauhan**, *Org. Lett.* **2023**, 25, 7523-7528.

Bio-Sketch of the Speaker

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Research Career

1. Associate Professor at IIT Jammu (August 2023-till date)
2. Assistant Professor at IIT Jammu (October 2017-August 2023)
3. Sub-Group Leader with Prof. Dieter Enders at RWTH Aachen University, Germany (April 2014- September 2017).
4. Postdoctoral Researcher with Prof. Dieter Enders at RWTH Aachen University, Germany (April 2013-March 2014).
5. Research Associate with Prof. Swapandeep Singh Chimni at Guru Nanak Dev University, Amritsar, India (November 2012-March 2013).
6. Ph.D. from Guru Nanak Dev University, Amritsar (November 2007-November 2012)

Research Interest

Asymmetric Synthesis, Organocatalysis, Photochemical and Electrochemical Organic Synthesis, Synergistic Catalysis, Domino/Cascade Reactions.

Awards and Recognitions

1. Selected for Chemical Research Society of India (CRSI) Bronze Medal, 2026.
2. Indian National Science Academy (INSA) Young Associate in 2024
3. Chirantan Rasayan Sanstha (CRS) Bronze Medal in 2024
4. RSC Research Fund (2022)
5. Thieme Journal Award (2018)
6. DST INSPIRE Faculty Award (2016).

Publications in Journals & Patents

Total publications: >80

Details of projects handled

Total projects: 5 Projects the funding agencies like ANRF, CSIR, RSC, JKSTIC, etc.

OL4

Supramolecular Ion Pair Adducts Favours Radical Excited State Cascade Electron Transfer for Chromoselective CO₂ Photoreduction

Kumari Raksha¹, Noufal Kandoth^{*1,2}

¹ Department of Chemical Sciences, Indian Institute of Science Education and Research-IISER Kolkata, Mohanpur, West Bengal, India

² School Chemical Science, Mahatma Gandhi University, Kottayam, Kerala, India

Abstract:

The charge transfer reactions are key to energy transformation in natural photosynthetic processes and various artificial catalytic transformations. Also, regulating photoinduced multi-electron/proton transfer across orders of magnitude in space and time is an overarching goal for such transformations. The recent research emphasis to achieve this is through custom engineered supramolecular architecture. We present herein a supramolecular nano-ensemble with a near spherical morphology (average diameter ~ 220 nm), comprising of a donor component, rhodamine B as a photosensitizer (PS) and an acceptor component, Co-based catalyst for the effective reduction of CO₂. Composition, morphology and optical properties of these nanoassemblies were established with appropriate spectroscopic, analytical and microscopic studies. These donor-acceptor catalytic components are synced through a dynamic contact ion pairing and stabilized by suitable counterions. Under 1 Sun illumination, the respective assembly selectively and efficiently induce syngas formation with appropriate reductants, and results also methane generation while involving radical anion excited states of PS upon chromoselective dual light activation. The quantitative analysis of CO₂ reduction products under single photon illumination generates ~377 μmol of syngas. Whereas the dual, orthogonal light exposure to the same system yielded ~212 μmol of syngas and an additional ~48 μmol of methane, underscoring the selectivity achieved through the formation of radical anion excited states. The microscopy, *in situ* optical and impedance spectroscopy, and mass spectrometry reveal a counter ion-driven ion-paired core-shell assembly that promotes photoinduced hopping electron transfer and radical anion excited state formation. Photoreduction of CO₂ to methane and syngas with this supramolecular architecture marks a level of selectivity rarely achieved in prior photocatalytic systems.

References:

- [1] O. S. Wenger *et al.*, *Nat. Commun.* 15 (1), 4738 (2024).
- [2] N. Kandoth *et al.*, *Sustain. Energ. Fuels*, 5 (3), 638 (2020).

CONTACT/PRESENTING AUTHOR

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Bio-Sketch of the Speaker

Noufal Kandoth

Associate Professor: School of Chemical Science,
Mahatma Gandhi University, Kottayam, Kerala, India



Research Career:

Associate Professor: School of Chemical Science, Mahatma Gandhi University, Kottayam, Kerala, India (Inorganic chemistry)
Research Assistant Professor: SRM IST Kattankulathur, Chennai, India (Photobiocatalysis)
SRA Pool Scientist (Prof. Amitava Das): IISER Kolkata, India (Inorganic nanomaterials/assemblies for nanomedicine)
Postdoc Research (Prof. J. Lloret-Fillol): ICIQ, Barcelona Institute of Science and Tech., Tarragona, Spain (Inorganic photochemistry, solar fuels)
Assistant Professor: National Institute of Technology, Karnataka, India 2015
Postdoc Research (Prof. Mauro Freccero): ISOF, National Research Council, Bologna, Italy 2015-2014
Doctoral Research (FP7-ITN Early-Stage Researcher): University of Catania, Italy 2012-2009
Marie Curie Early-Stage Researcher: University of Catania, Italy 2013-2010
Project Intern: Mahatma Gandhi University, Kerala, India 2010
Master Research Intern: Bhabha Atomic Research Center (B.A.R.C), India 2009-2008
Authored 34 publications (13 first authorship) in international peer reviewed journals (ACS, RSC, Wiley).

Research interests: Photochemistry, Supramolecular chemistry, Material chemistry

Awards and Scholarship

2025- ANRF Early Career Research Grant by ANRF India, ~55 Lakhs.
2020- CSIR SRA-Scientist Pool Scheme, IISER Kolkata, India.
2020- Marie Skłodowska-Curie Actions, Zeal of Excellence for the IF proposal 2019 (91/100).
2020-2018- Juan de la Cierva Fellowship for doing Postdoc research at ICIQ, Tarragona, Spain.
2018- Best Poster Prize, Photo4Future: Symposium on Photochemistry, 12-14 November 2018, Eindhoven University of Technology, Netherlands.
2017-2015- ERC Fellowship for doing Postdoc at ICIQ, Tarragona, Spain.
2014- EPA PhD prize for the best doctoral thesis in the European photochemistry: Runners up.
2013-2012- Elected as mentor and tutor for the undergraduate students in Biomolecular chemistry at Elected as mentor and tutor for the undergraduate students in Biomolecular chemistry at University of Catania, Italy.
2010-2013- Marie Curie Initial Training Networks, ITN (Cyclon/No. 237962, FP7-PEOPLE-ITN-2008, E. U.) Scholarship for doing PhD in chemical science.
2009- National scholarship (funded by Indian Academy of Sciences) for summer research carried out at B.A.R.C., Mumbai, India

IL12

Chemical Tools for Glycobiology

Valentin Wittmann

Department of Chemistry, University of Konstanz, 78457 Konstanz, Germany.

Abstract:

The elucidation of the numerous biological functions of carbohydrates benefits enormously from the development of chemical tools designed to achieve tight binding of carbohydrates to proteins and RNA, to synthesize glycoconjugates, and to trace carbohydrates within cells. This lecture will give an overview of some of our achievements in these fields.

We synthesized numerous high-affinity **multivalent lectin ligands** including a photoswitchable one^[1] and developed a new design of multivalent lectin ligands, termed inline lectin ligands (iLecs).^[2] iLecs lead to exceptionally high binding affinities without concurrent precipitation of proteins due to crosslinking. **RNA-binding carbohydrates** derived from glucosamine-6-phosphate (GlcN6P) can function as activators of the *glmS* riboswitch and are promising lead structures for the development of future antibiotics with a potentially novel mode of action.^[3]

Conjugation of unprotected (reducing) carbohydrates to surfaces or probes by **chemoselective ligation reactions** is indispensable for the elucidation of their biological functions. We studied the kinetics of the oxyamine ligation by real-time NMR spectroscopy and could show that the reaction rate is significantly increased (up to 500-fold) without the need for a catalyst when starting with glycosyl amines.^[4]

Metabolic glycoengineering (MGE) is now a well-established approach to study the biological roles of carbohydrates.^[5] We applied the inverse-electron-demand Diels-Alder (IEDDA) reaction in MGE to achieve the visualization of protein-specific glycosylation within living cells using confocal FLIM-FRET microscopy. To study protein-O-GlcNAcylation, we developed dienophile-modified glucosamine-1-phosphate derivatives that do not lead to non-specific labeling by the recently reported S-glyco modification.^[6]

References:

- [1] U. Osswald, J. Boneberg, V. Wittmann, *Chem. Eur. J.* **2022**, *28*, e202200267.
- [2] P. Rohse, S. Weickert, M. Drescher, V. Wittmann, *Chem. Sci.* **2020**, *11*, 5227-5237.
- [3] B. Silkenath, D. Kläge, P. Eppelin, J. S. Hartig, V. Wittmann, *J. Org. Chem.* **2025**, *90*, 2969-2977.
- [4] M. A. Rapp, O. R. Baudendistel, U. E. Steiner, V. Wittmann, *Chem. Sci.* **2021**, *12*, 14901-14906.
- [5] M. Kufleitner, L. M. Haiber, V. Wittmann, *Chem. Soc. Rev.* **2023**, *52*, 510-535.
- [6] M. Kufleitner, L. M. Haiber, S. Li, H. Surendran, T. U. Mayer, A. Zumbusch, V. Wittmann, *Angew. Chem., Int. Ed.* **2024**, *63*, e202320247.

Bio-Sketch of the Speaker

Prof. Dr. Valentin Wittmann

University of Konstanz
Department of Chemistry
Universitätsstr. 10
78457 Konstanz, Germany
E-mail: Valentin.Wittmann@uni-konstanz.de
www.valentin-wittmann.de



Research Career

Valentin Wittmann studied Chemistry at the Goethe-University of Frankfurt (Germany). In 1994 he obtained a PhD from the Technical University of Munich (Germany) for his work on C-glycopeptides under the supervision of Prof. Horst Kessler. Subsequently, he carried out postdoctoral research with Prof. Christian Griesinger at the Goethe-University of Frankfurt (Germany) in the field of stable-isotope-labeled oligonucleotides and with Prof. Chi-Huey Wong at The Scripps Research Institute in La Jolla, California (USA) working on the chemoenzymatic synthesis of oligosaccharides. In 1997 he returned to Frankfurt to start independent research. Since 2003 he is professor of organic/bioorganic chemistry at the University of Konstanz (Germany). From 2006 until 2011 he was Dean of Studies, from 2016 until 2020 and from 2024 until 2025 head of the Department of Chemistry, and from 2016 until 2023 vice coordinator of the Collaborative Research Center SFB 969.

Research Interest

Chemical biology of carbohydrates, metabolic glycoengineering, investigation of multivalent carbohydrate-protein interactions, development of ligation reactions, glycopeptide synthesis, RNA-targeting antibiotics

Awards and Recognitions

2012, 2016, 2020 Teaching Award "Lehrpreis der Universität Konstanz von Studierenden (LUKS)"
2009 Lectureship Award, sponsored by the National Science Council of Taiwan
2001 SYNTHESIS-SYNLETT-Journals Award
2000 Adolf Messer Prize for interdisciplinary research
1998 – 1999 Habilitation scholarship of the Deutsche Forschungsgemeinschaft
1995 – 1996 Research fellowship of the Deutsche Forschungsgemeinschaft
1990 – 1992 Scholarship for Ph.D. students of the Fonds der Chemischen Industrie

Recent Publications in Journals

- M. Kufleitner, L. M. Haiber, S. Li, H. Surendran, T. U. Mayer, A. Zumbusch, V. Wittmann. Next-Generation Metabolic Glycosylation Reporters Enable Detection of Protein O-GlcNAcylation in Living Cells without S-Glyco Modification. *Angew. Chem., Int. Ed.* 2024, 63, e202320247.
- M. Kufleitner, L. M. Haiber, V. Wittmann. Metabolic Glycoengineering – Exploring Glycosylation with Bioorthogonal Chemistry. *Chem. Soc. Rev.* 2023, 52, 510-535.
- M. A. Rapp, O. R. Baudendistel, U. E. Steiner, V. Wittmann. Rapid Glycoconjugation with Glycosyl Amines. *Chem. Sci.* 2021, 12, 14901-14906.
- P. Rohse, S. Weickert, M. Drescher, V. Wittmann. Precipitation-Free High-Affinity Multivalent Binding by Inline Lectin Ligands. *Chem. Sci.* 2020, 11, 5227-5237.

SL10

Glycosyl Thiosulfonate-Enabled *Ortho*-Thiolation via the Catellani Strategy: A Modular Synthesis of Polysubstituted Aryl Thioglycosides

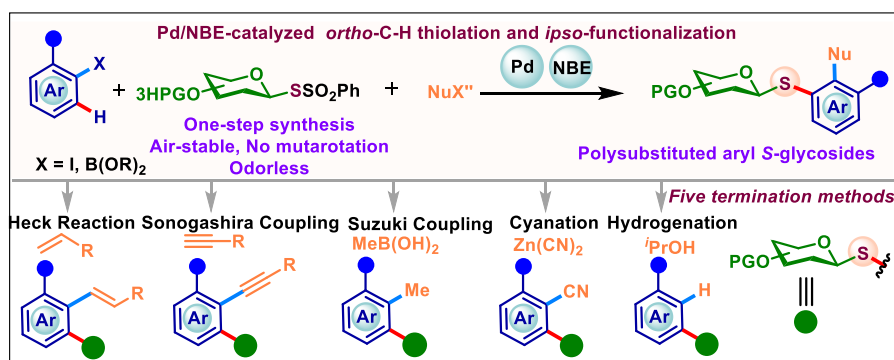
Dr Pintu Kumar Mandal^{1,2*}, Zanjila Azeem^{1,2}

¹ Medicinal & Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow 226031, India.

² Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India.

Abstract:

Site-selective introduction of a glycosylthiol group into aromatic compounds is a crucial process in organic chemistry. However, the position that a glycosylthiol moiety can be introduced to is largely restricted to a pre-functionalized site; otherwise, electronically biased substrates or auxiliary groups are needed. Moreover, common ways to prepare stereoselective aryl thioglycosides often rely on cross-coupling reactions between aryl halides and glycosylthiols. These methods form carbon–sulfur (C–S) bonds at the *ipso* position of aryl halides; thus, the position of the installed sulfur moiety is restricted by the position of the halide. Switching *ipso* to *ortho* thiolation is a formidable challenge and has not yet been reported in sugar chemistry. In this study, we introduce for the first time a modular approach involving glycosyl thiosulfonate-enabled *ortho*-C–H thioglycosylation and *ipso*-functionalization of aryl iodides/boron via palladium/norbornene cooperative catalysis.



References:

[1] Z. Azeem, S. Maurya, A. K. Gupta, Shalini, R. Kant, P. K. Mandal, *Chem. Commun.*, 61, 15634 (2025).

Bio-Sketch of the Speaker

Dr. Pintu Kumar Mandal

Professor of Chemical Sciences, AcSIR
Senior Principal Scientist
Medicinal and Process Chemistry Division
CSIR-Central Drug Research Institute
Lucknow-226031
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E-mail: pintuchem06@gmail.com/pk.mandal@cdri.res.in



Research Career

Pintu Kumar Mandal obtained Ph.D. in 2009 at the Jadavpur University (Bose Institute), Kolkata, he pursued his postdoctoral research in the laboratory of Professor W. Bruce Turnbull at the University of Leeds, Leeds. He was selected as a Newton International Fellow (RSC, 2009–2011) at the University of Leeds, UK. Then, he moved to the Georgia State University, Atlanta, USA to work with Professor Peng George Wang. He returned back to India in May, 2013 and held a Senior Scientist position, currently holds the position of Senior Principal Scientist at CSIR-CDRI, Lucknow. His research interests include the efficient chemical synthesis of biologically relevant *N*-, *S*-, *O*- or *C*-glycosides and catalytic stereoselective glycosylation and functionalization.

Research Interest

Transition metal-catalyzed approaches to explore new ways to functionalize glycosides and the development of a series of processes concerning *N*-, *S*-, *O*- or *C*-glycosidic bonds functionalization as well as focuses on organocatalytic stereoselective glycosylation, glycan synthesis.

Awards and Recognitions

ACCT(I) Dr. H C Srivastava Memorial Award-2025
ACCT(I) C.G. Merchant Memorial Award-2023
Newton International Fellow (Royal Society of Chemistry, 2009-2011)

Publications in Journals & Patents

Publication: 80
Book chapter: 2

Details of projects handled

Projects: 5

SL11

Molecular Insights into Lectin Architecture and Glycan Specificity in *Photorhabdus* spp.

Michaela Wimmerova^{1,2*}

¹ National Centre for Biomolecular Research, Faculty of Science, Masaryk University, Kotlarska 2, 61137 Brno, Czech Republic

² Central European Institute of Technology, Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic

Abstract:

Lectins are non-immune carbohydrate-binding proteins that mediate diverse recognition processes in host–microbe interactions. Members of the genus *Photorhabdus*, which exist in mutualistic association with *Heterorhabditis* nematodes and act as pathogenic agents toward insect (and in some cases, human) hosts, produce a wide variety of lectins implicated in both symbiosis and virulence.

Our work focuses on the discovery, structural elucidation, and functional characterization of *Photorhabdus* lectins, including lectin families or examples, e.g., β -propeller (PLLs) or TNF-like (PLTL). These proteins display key structural or biochemical features, e.g., diverse oligomeric states, unusual binding-site organization, or high specificity for fucosylated and O-methylated glycans], suggesting specialized biological roles.

We employ a multidisciplinary approach combining methods such as X-ray crystallography, calorimetry, surface plasmon resonance, and glycan arrays to investigate carbohydrate recognition, protein assembly, and their potential influence on host immune modulation, bacterial adhesion, or symbiotic colonization.

In parallel, synthetic carbohydrate ligands or inhibitors—including polyvalent and chemically stabilized derivatives—are evaluated to probe binding mechanisms and explore their inhibitory potential.

Overall, this research integrates structural, biochemical, and chemical glycoscience perspectives to advance our understanding of lectin-mediated recognition processes in *Photorhabdus* spp. and their broader relevance to host–pathogen and host–symbiont interactions.

References:

- [1] F. Melicher, P. Dobes *et al*, *FEBS J*, Oct2025(Early Access)
- [2] E. Paulenova, P. Dobes *et al*, *Glycobiology*35, cwaf033 (2025).
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CONTACT/PRESENTING AUTHOR

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Bio-Sketch of the Speaker

Prof. Michaela Wimmerova

Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic

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Michaela Wimmerová is a Professor at Masaryk University (MU), Brno, Czech Republic, and Head of the Glycobiology Research Group at the Central European Institute of Technology (CEITEC MU). Since 2022, she has also served as Director of the National Centre for Biomolecular Research (NCBR) at the Faculty of Science, MU. She obtained her PhD in Biochemistry from Masaryk University in 1996 and subsequently spent a research stay at the Centre de Recherches sur les Macromolécules Végétales (CERMAV), CNRS, in Grenoble, France. Upon returning to Brno, she established the Glycobiology Research Group, focusing on proteins involved in host–pathogen recognition. Prof. Wimmerová also founded and led the Biomolecular Interactions and Crystallization Core Facility at CEITEC MU, equipping it with cutting-edge instrumentation for advanced biophysical analyses. She is an active member of the national and international scientific community, serving on the board of the Czech Society for Biochemistry and Molecular Biology and representing the Czech Republic in the International Glycoconjugate Organisation. Her research expertise spans protein biochemistry, molecular biology, and structural glycobiology, with a focus on protein–carbohydrate interactions and host–pathogen recognition. Her group has identified and characterized several novel lectins and other carbohydrate-binding proteins with unique structural and functional properties.

Research Career

2022 – till now Director, National Centre for Biomolecular Research, Masaryk University, Brno, Czech Republic

2013 – till now Professor, Masaryk University, Brno, Czech Republic

2011 – 2021 Head of Biomolecular Interactions and Crystallization Core Facility, CEITEC MU Brno, Czech Republic

2011 – till now Group leader, Central European Institute of Technology, Masaryk University, Brno, Czech Republic

2007 – 2013 Associate Professor, Masaryk University, Brno, Czech Republic

2001-2002 Centre de Recherches sur les Macromolécules Végétales (CERMAV), CNRS, Grenoble, France

2001 – till now Group leader, National Centre for Biomolecular Research, Masaryk University, Brno, Czech Republic

1996-2007 Assistant Professor, Masaryk University Brno, Czech Republic

1991 – 1996 Researcher, Masaryk University Brno, Czech Republic

1996 Ph.D. Masaryk University, Brno, Czech Republic (Biochemistry)

Awards and Recognitions

2022 – member of the Scientific Board of the Faculty of Science, Masaryk University

2015 -2019 the Association of Resources for Biophysical Research in Europe, elected as Management

2011 – 2014, 2017 – 2022 Czech Science Foundation, Member of the Evaluation Committee

2011 – till now National representative in International Glycoconjugate Organisation (IGO)

2011 – till now Glycobiology, Member of the Editorial board

2010 – 2013 Federation of European Biochemical Societies (FEBS), Fellowships Committee

2007 – till now vice-president of the National Board of Czech Society for Biochemistry and Molecular Biology

Publications in Journals & Patents 102

Details of projects handled More than 30

SL12

Chemical Biology of Bacterial c-di-GMP Signaling

Dr. Dimpy Kalia

Department of Chemistry

Indian Institute of Science Education and Research (IISER) Bhopal, India

(dimpy@iiserb.ac.in)

Research in my laboratory lies at the chemistry–biology interface and utilizes organic chemistry to address questions of biological importance. The two main areas of research that my laboratory focuses on are: protein bioconjugation and the chemical biology of the bacterial second messenger c-di-GMP.

In this talk, I will describe our most recent work on c-di-GMP—a key signaling molecule which regulates several aspects of bacterial physiology, including biofilm formation, virulence, exopolysaccharide production, and cellular motility.¹ I shall discuss the chemoproteomic platform that we have developed for the discovery of the c-di-GMP-interacting proteome of bacterial cells², and shall also describe our efforts towards the development of selective inhibitors of c-di-GMP synthases³. Additionally, I will highlight key chemical approaches that my laboratory has developed over the years for highly efficient protein bioconjugation^{4–7}, including our Baylis Hillman orchestrated Protein Amino-thiol Labelling (BHoPAL) technology that enables rapid and quantitative labelling of any desired site on any protein with stoichiometric, low-micromolar protein and labelling reagent concentrations⁴.

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<https://pubs.rsc.org/en/content/articlelanding/2013/cs/c2cs35206k>
2. Veena S. Anwani, Sangeeta Parmar and Dimpy Kalia*. Photocrosslinkable c-di-GMP analogs for chemoproteomic applications, *Manuscript under preparation*.
3. Chhaya Singh, Deepa Gond, Fabina K. Binth and Dimpy Kalia*, Development of targeted covalent inhibitors of the bacterial cyclic-di-GMP synthase, WspR, and their use for inhibitor screening, *Manuscript under preparation*.
4. Mudassir H. Mir†, Sangeeta Parmar†, Chhaya Singh, Dimpy Kalia* (†equal contribution). *Nat. Commun.*, **2024**, 15, 859. <https://www.nature.com/articles/s41467-024-45124-2>
5. Dimpy Kalia*, Pushpa V. Malekar and Manikandan Parthasarathy. *Angew. Chem. Int. Ed. Engl.*, **2016**, 55, 1432–1435. (Very Important Paper). <https://onlinelibrary.wiley.com/doi/10.1002/anie.201508118>
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7. Sangeeta Parmar, Sharad P. Pawar, Ramkumar Iyer and Dimpy Kalia* *Chem. Commun.*, **2019**, 55, 14926–4929.
<https://pubs.rsc.org/en/content/articlelanding/2019/cc/c9cc07443k>

Bio-Sketch of the Speaker

Dr. Dimpy Kalia

Chemical Biology

Assistant Professor

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Dimpy was born and raised in Chandigarh (India). She completed her M.Sc. (Hons.) in Chemistry from Panjab University (Chandigarh) in 2004 and subsequently joined Aurigene Discovery Technologies Ltd. (Bangalore) where she worked as a synthetic organic chemist. After spending a little over a year at Aurigene, Dimpy joined CDRI Lucknow to pursue her Ph.D. under the guidance of Dr. Dinesh K. Dikshit. Her Ph.D. research focused on organic synthesis, specifically on natural product synthesis and on the synthesis of anti-tubercular compounds. After completing her Ph.D. in 2011, Dimpy began her second stint at Aurigene and worked there for a year. She worked at IISER Pune for six months as an IISER Fellow in 2013 before moving to the Department of Chemistry at the Savitribai Phule Pune University (SPPU) as a DST-INSPIRE faculty to start her independent research and teaching career. At SPPU, Dimpy's lab focused primarily on developing facile chemistry for thiol bioconjugation. In 2018, she moved to the Department of Chemistry at IISER Bhopal as an Assistant Professor. In addition to science, Dimpy enjoys going for long runs and spending time with family.

Research Interest

Developing facile approaches of protein bioconjugation, chemical biology of c-di-GMP signaling in bacteria, and developing new concise methods for the synthesis of complex heterocyclic small molecules.

Day 2 – 18-11-2025, Auditorium 1

Online IL13

Site-Selective Aliphatic C—H Oxidations

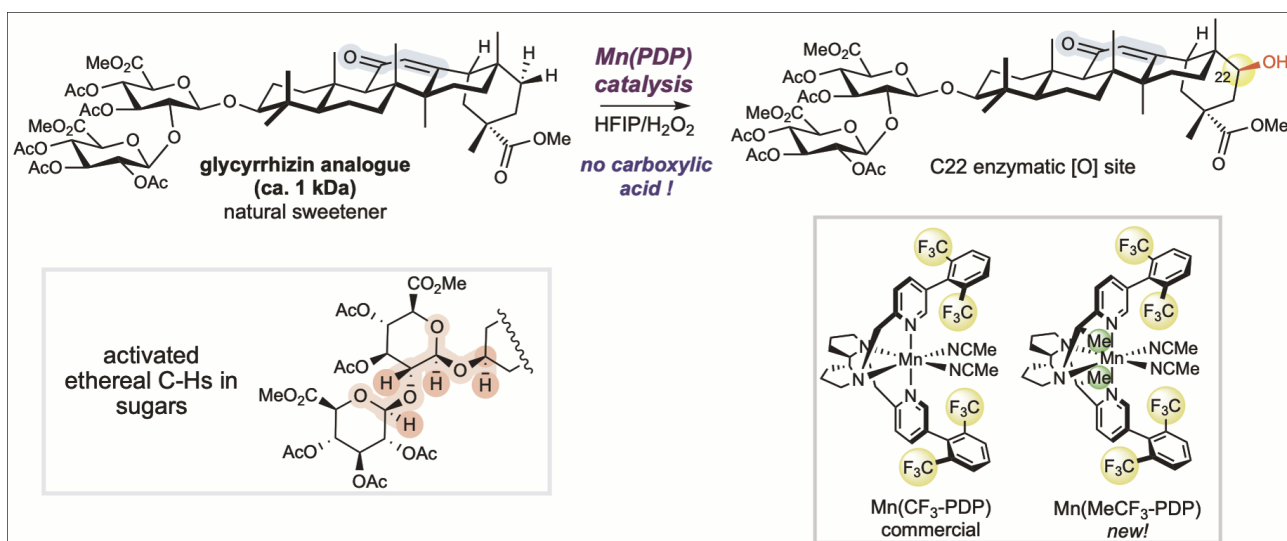
M Chritina White

Dept. of Chemistry, University of Illinois

Roger Adams Laboratory; Box 58-5 600 South Mathews Avenue Urbana, IL 61801

email: mcwhite7@illinois.edu

Abstract:



Bio-Sketch of the Speaker

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Lycan Professor of Chemistry

Dept. of Chemistry

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Urbana, IL 61801

Web site <http://www.scs.illinois.edu/white/>



M. Christina White was born in Athens, Greece. She received a B.A. degree with highest honors in biochemistry from Smith College working with Stuart Rosenfeld in the area of host-guest chemistry. After a one-year stint in the biology graduate program working with Christian Anfinsen on thermophilic bacteria protein folding, she received her Ph. D. degree from Johns Hopkins University in chemistry with Gary Posner as an ACS Medicinal Chemistry Pre-Doctoral fellow. She was a NIH postdoctoral fellow at Harvard University with Eric Jacobsen from 1999-2002 and is currently the Lycan Professor of Chemistry at the University of Illinois at Urbana-Champaign. The White group's reactions have enabled strategic advances in synthesis, most notably the concept of late-stage C—H functionalization. The White group discovers and develops selective, intermolecular C—H oxidation reactions for broad use in chemical synthesis. They have contributed new reactions to intermolecularly functionalize all types of C(sp³)—H bonds under preparative conditions with predictable and catalyst-controlled site-selectivities - without the requirement for directing groups. The White group has commercialized 5 catalysts that are broadly used academically and industrially to add oxygen, nitrogen and carbon to preformed hydrocarbon skeletons in every class of natural product and emerging classes of pharmaceuticals. These reactions provide fundamental insights into the selective reactivity possible among C—H bonds of the same bond type (for example, methylenes) based on subtle differences in their electronics, sterics, stereoelectronic environments in complex settings.

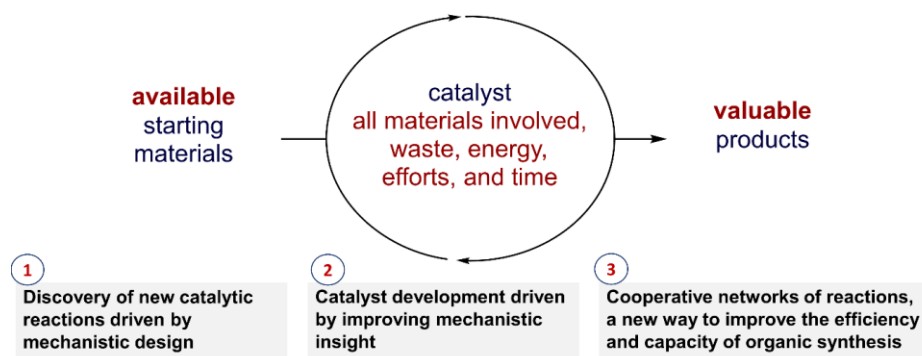
IL14

Unlocking Chemical Innovation Through Mechanistic Design and Multicatalysis

Pawel Dydio

*Yusuf Hamied Department of Chemistry, University of Cambridge,
Lensfield Rd, Cambridge CB2 1EW, United Kingdom*

Catalysis lies at the heart of chemical innovation, enabling cleaner technologies, improving the material and energy efficiency of processes, and unlocking the potential of renewable feedstocks.^[1]



In this seminar, I will present our group's research in catalytic chemistry, shaped by these challenges and opportunities. Our approach is founded on three interrelated strategies: (1) the development of new organic transformations through mechanistic design;^[2,3] (2) catalyst development guided by detailed mechanistic understanding;^[4,5] and (3) the creation of complex transformations through relay multicatalysis.^[6–11]

Each of these strategies will be illustrated through recent examples, highlighting not only the synthetic utility but also the broader conceptual advances. I will also outline our ongoing efforts aimed at further expanding the reach of catalysis in chemical synthesis.

- [1] L. Veth, P. Dydio, *Nat. Chem.* **2022**, *14*, 1088–1088.
- [2] L. Veth, H. A. Grab, S. Martínez, C. Antheaume, P. Dydio, *Chem Catal.* **2022**, *2*, 762–778.
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Bio-Sketch of the Speaker

Research Career

- Yusuf Hamied Department of Chemistry, University of Cambridge, UK
University Assistant Professor (October 2023 – present)
- Institut de Science et d'Ingénierie Supramoléculaires (ISIS), Université de Strasbourg, France
Professeur conventionné (October 2023 – present)
Assistant Professor of Chemistry (Maître de Conférences Associé) and Director of Laboratoire des Systèmes Complexes en Synthèse et Catalyse (August 2016 - September 2023)
- Department of Chemistry, University of California, Berkeley, USA
NWO Rubicon postdoctoral fellow (June 2014 – June 2016)
LBNL postdoctoral fellow (February 2014 – June 2014)
PD advisor: Prof. Dr. John F. Hartwig
- HIMS, University of Amsterdam, Amsterdam, The Netherlands
NRSCC Doctoral scholar (July 2009 – June 2013)
PhD advisor: Prof. Dr. Joost N. H. Reek
- Institute of Organic Chemistry, PAS, Warsaw, Poland
Predoctoral research fellow (November 2008 – June 2009)
Advisor: Prof. Dr. Janusz Jurczak
- University of Warsaw, Warsaw, Poland
M.Sc. Student (October 2004 – June 2009)



Awards:

- *Thieme Chemistry Journals Award (2023)*
- *Guy Ourisson Prize the Gutenberg Circle (2021)*
- *Dream Chemistry Award Top 5 (2020)*
- *Bürgenstock JSP Fellow (2020)*
- *ERC Starting Grant 2018 Awardee*
- *Chaire attractivité Recherche 2016* – Junior Chair of the framework Excellence Initiative of the University of Strasbourg
- *NWO Rubicon fellow* (competitive postdoctoral fellowship, equivalent of Marie Curie Actions Program), awarded by The Netherlands Organization for Scientific Research (NWO) for 2 years (2014-2016)
- *LBNL Postdoctoral fellow* and affiliate (2014-2016)
- *PhD Cum laude* – the highest PhD honors at U. Amsterdam (2013);
- *MSc Suma cum laude* – the highest MSc honors at U. Warsaw (2008);
- *Gold Medal Winner* at International Chemistry Olympiad, Germany (2004);
- *Fellowship* of the Polish Children's Fund (2002-2004);
- *Scholarships* of the Polish Ministry of Science and Higher Education (2005-2008), the Polish Minister of National Education (2004) and the Prime Minister of the Polish Government (2002-2004).

IL15

Guanosine at the Crossroads of Chemistry and Biology

Jyotirmayee Dash*¹¹ Indian Association for the Cultivation of Science, Kolkata, School of Chemical Sciences, Jadavpur, 700032, India.**Abstract:**

Guanosine, a naturally occurring nucleobase, serves as a molecular bridge between chemistry and biology through its exceptional ability to self-assemble via Hoogsteen hydrogen bonding and metal ion coordination. The resulting G-quartets stack into higher-order architectures that form the foundation of both synthetic supramolecular systems and naturally occurring nucleic acid quadruplexes.^[1] In the chemical domain, such assemblies give rise to functional soft materials, including guanosine-derived hydrogels and membrane-spanning ion channels, which mimic biological transporters and catalyze chemical transformations. These hydrogels facilitate in situ generation of DNA-binding ligands, while guanosine-based ion channels enable selective metal-ion and drug transport.^[2] Biologically, the G-quartet motif forms the structural core of DNA and RNA G-quadruplexes, which regulate oncogene expression (*c-KIT*, *KRAS*, *c-MYC*).^[3] Chemical modulation of these quadruplex structures through rational design and target-guided synthesis provides powerful strategies for therapeutic intervention.^[4] The talk will highlight how guanosine self-assembly integrates principles of supramolecular chemistry, nucleic acid biology, and molecular medicine to inspire next-generation biomimetic and therapeutic systems.

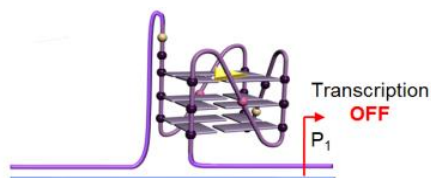


Figure 1. Gene regulation through DNA G-quadruplex.

References:

- [1] P. Saha, D. Panda, J. Dash, *Chem. Soc. Rev.* 52, 4248-4291 (2023).
- [2] Y. P. Kumar, M. Debnath, T. Das, R. Paul, J. Dash, *Cell Rep. Phys. Sc.* 5, 102298 (2024).
- [3] T. Bhattacharyya, S. Pal, S. Pradhan, J. Dash, *J. Med. Chem.* 68, 20060–20080 (2025).
- [4] R. Chaudhuri, P. Thumapati, J. Dash, *Angew. Chem. Int. Ed.* 62, e202215245 (2023).

Bio-Sketch of the Speaker

Prof. Jyotirmayee Dash

Senior Professor

Indian Association for the Cultivation of Science, Kolkata

School of Chemical Sciences, Jadavpur, 700032

Homepage:

<http://iacs.res.in/athusers/index.php?navid=0&userid=IACS0034>



Phone No.: 8910218626, 9635350592

E-mail: ocjd@iacs.res.in

Research Career

Professor Jyotirmayee Dash obtained her Ph.D. in Organic Chemistry from the Indian Institute of Technology (IIT) Kanpur, India. She was awarded the Alexander von Humboldt Fellowship at Freie Universität Berlin, a postdoctoral fellowship at ESPCI Paris, and the Marie Curie Fellowship at the University of Cambridge, UK. She joined IISER Kolkata as an Assistant Professor in 2009 and is currently a Senior Professor at the Indian Association for the Cultivation of Science (IACS), Kolkata.

Research Interest

Her research interests span new organic transformations, supramolecular chemistry, and the structure and function of nucleic acids.

Awards and Recognitions

She has received several prestigious recognitions, including the DST Swarnajayanti Fellowship (2015–2016), DBT Wellcome Trust Fellowship (2020), Shanti Swarup Bhatnagar Prize (2020), and the Bronze Medal of the Chemical Research Society of India (2020). She is an elected Fellow of the Indian Academy of Sciences (IASc, 2021) and the National Academy of Sciences, India (NASI, 2025). Professor Dash serves on the Advisory Boards of *ACS Bioconjugate Chemistry*, *ACS Omega*, *Asian Journal of Organic Chemistry*, and *Chemical Communications*, and as an Editor of *Bioorganic & Medicinal Chemistry Letters* and the *Journal of the Indian Chemical Society*.

Publications in Journals & Patents

150

Details of projects handled

12

IL16

Unlocking new chemical space via selective catalysis

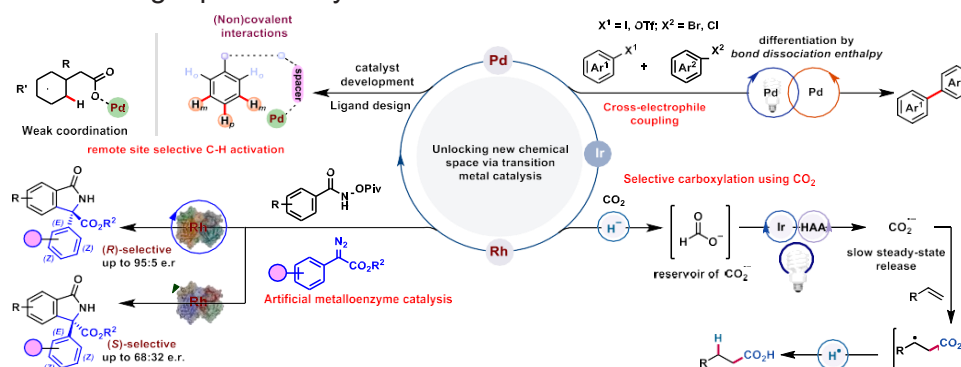
Debabrata Maiti

Department of Chemistry, IIT Bombay, www.dmaiti.com,

Email : dmaiti@iitb.ac.in

Abstract:

The limitations of cross-coupling such as the availability of prefunctionalized coupling partners, instability, and synthesis expense remain, posing significant barriers to unlocking new chemical space for molecular complexity. To solve these underlying problems of cross-coupling we are mainly focused on the development of techniques for direct C–H functionalization and cross- electrophile coupling. Selectively targeting a remote C–H bond in a molecule remains more challenging due to the inaccessibility of these sites in formation of energetically favorable organometallic pre-transition states. We believe that the direct release of the reactive metal catalyst in close proximity to the targeted remote C–H bond could solve this problem. We devised covalently attached template-directed methods that require precise spatial positioning of the directing group in order to selectively activate remote C–H bonds. We recently demonstrated that various non-covalent interactions are also successful in recognizing the perfect orientation of catalyst and the substrate to achieve selective C–H bond activation. In this vein, we have developed a method for the activation of methylene C–H bond in presence of methyl C–H bonds to form unsaturated bicyclic lactones utilizing the weak coordinating nature carboxylic acid towards palladium. Cross-electrophile coupling (XEC) approach would be a powerful tool for the construction of (hetero)biaryl moiety because of the widespread availability and stability of (hetero)aryl electrophiles. We have demonstrated a ligand controlled visible light driven monometallic cross-electrophile coupling platform for the synthesis of unsymmetrical (hetero)biaryls directly from (hetero)aryl halides and pseudohalides. In addition, our lab is pursuing the development of a paradigm in which small molecules such CO₂, SO₂ etc. can be converted into a wide range of chemicals and materials using renewable visible light photocatalysis.

**References**

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2. Goswami, N.; Sinha, S. K.; Mondal, P.; Adhya, S.; Datta, A.; Maiti, D. *Chem*, **2023**, 9, 989.

3. Saha, A.; Guin, S.; Ali, W.; Bhattacharya, T.; Sasmal, S.; Goswami, N.; Prakash, G.; Sinha, S. K.; Chandrashekar, H. B.; Panda, S.; Anjana, S. S.; Maiti, D. *J. Am. Chem. Soc.* **2022**, *144*, 1929.
4. Das, J.; Ali, W.; Ghosh, A.; Pal, T.; Mandal, A.; Teja, C.; Dutta, S.; Pothikumar, R.; Ge, H.; Zhang, X.; Maiti, D. *Nat. Chem.* **2023**, *15*, 1626.
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6. Mukherjee, P.; Sairaman, A.; Deka, H. J.; Jain, S.; Mishra, S. K.; Roy, S.; Bhaumik, P.; Maiti, D. *Nat. Synth.* **2024**

Bio-Sketch of the Speaker

Prof. Debabrata Maiti

Institute Chair Professor
Department of Chemistry
Indian Institute of Technology Bombay
Powai, Mumbai-400076, India
E-mail: dmaiti@chem.iitb.ac.in
dmaiti@iitb.ac.in



Prof. Debabrata Maiti received his PhD from Johns Hopkins University in 2008 under the supervision of Prof. Kenneth D. Karlin. After postdoctoral studies at MIT with Prof. Stephen L. Buchwald, he joined the Department of Chemistry at IIT Bombay in 2011. His research interests are focused on the development of new and sustainable synthetic and catalytic methodologies. Currently he is *Editor-in-Chief*, *Synlett*.

IL17

Machine Learning and Generative-AI for Chemical Reactions

Raghavan B. Sunoj

Department of Chemistry and
Centre for Machine Intelligence and Data Science,
Indian Institute of Technology Bombay, Mumbai 400076.

Abstract:

Increasing number of application of artificial intelligence and machine learning in almost all facets of life has appeared in recent years, including those in chemistry and biology.ⁱ The hype surrounding AI as a universal problem solver and the perceived threats of it replacing human experts from their jobs remain eerily close and realistic.ⁱⁱ Insofar as AI/ML adaptations to chemical space is concerned, most of such studies focused on molecular property predictions of significance to drug discovery. Similarly, generative-AI techniques have shown promise even in incredibly harder problems such as antibiotic discovery.ⁱⁱⁱ While dovetailing predictive abilities of ML with gen-AI seems to offer interestingly new avenues for molecular discovery, the feasibility of synthesis of such generated compounds would require careful assessment.

It should be reckoned that the reliability of an ML model depends on the training data and on the nature of the tasks that it is deployed to predict. One of the challenging applications of AI/ML is in predicting reaction outcome, such as the yield or selectivities.^{iv} If these outcomes can be predicted, time and resources could be saved before setting out to carry out reactions, which are likely to be poor yielding. This talk would highlight how ML models can be designed, even with a few hundreds of training data, and how it could be extended to molecular generation for reaction development.^v In particular, the utility of reinforcement learning to identify new substrates with improved yields or catalysts that can enhance enantioselectivity would be highlighted.^{vi} A critical and realistic evaluation of whether or not generative-AI might be able to guide future experimental exploration in the domain of asymmetric catalysis would as well be in focus.^{vii}

References:

- ¹ . Catherine, O. www.science.org/content/article/protein-designer-and-structure-solvers-win-chemistry-nobel (accessed 30 Sept. 2025).
- ¹ Frank, M. R. *Proc. Natl. Acad. Sci.* **2019**, *116*, 6531.
- ¹ Stokes et al. A Deep Learning Approach to Antibiotic Discovery. *Cell* **2020**, *180*, 688.
- ⁵ Singh, S.; Sunoj, R. B. *Acc. Chem. Res.*, **2023**, *56*, 402.
- ⁶ a) Singh, S.; Pareek, M.; Changotra, A.; Banerjee, S.; Bhaskararao, B.; Balamurugan, P.; Sunoj, R. B. *Proc. Natl. Acad. Sci.* **2020**, *117*, 1339. b) Das, M.; Sharma, P.; Sunoj, R. B. *J. Chem. Phys.* **2022**, *156*, 114303. c) Hoque, A.; Sunoj, R. B. *Digital Discovery* **2022**, *1*, 923. d) Ghosh, A.; Kashyap, G.; Mittal, S.; Jain, N.; Sunoj, R. B.; De, A. Learning Condensed Graph via Differentiable Atom Mapping for Reaction Yield Prediction. *International Conference on Machine Learning (ICML)*, **2025**.
- ⁷ Hoque, A.; Surve, M.; Kalyanakrishnan, S. Sunoj, R. B. *J. Am. Chem. Soc.* **2024**, *146*, 28250.
- ⁸ Hoque, A.; Chang, T.; Yu, J.-Q.; Sunoj, R. B. *Chem. Sci.* **2025**, *16*, 13276–13290.

Bio-Sketch of the Speaker

Raghavan B. Sunoj

Professor

Room 418A, Chemistry Bldg.

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+91 22 2576 7173



Research Career:

- Ph.D., Indian Institute of Science, Bangalore
- M.Sc., University of Kerala
- B.Sc., University of Kerala
- Professional Experience:
- Post-doc, The Ohio State University, USA
- Assistant Professor, IIT Bombay (2003)
- Associate Professor, IIT Bombay (2007)
- Professor, IIT Bombay (2012)

Research Interest:

We work on a range of problems in chemical reactivity, with particular emphasis on catalytic reactions and asymmetric transformations. To study the catalytic action, a combination of computational chemistry and machine learning methods are employed. Catalytic reaction of our current interest is cooperative multi-catalytic transformations involving two or more catalysts. We examine such reactions by identifying various intermediates and transition states along the reaction path from reactants to products. Molecular insights, such as the weak interactions in the transition state, are subsequently employed for predicting new catalyst/reactions. Good number of examples on noncovalent interaction (NCI) driven asymmetric catalysis have been reported by group. Another domain of our active research efforts is in the use of machine learning (ML) for chemical catalysis. We aim to identify optimal reaction conditions to maximize the yield and selectivity, in relatively small data settings. The ML models are trained to predict reaction outcomes (yield, enantio-, regio-selectivities). Reliable models, built on various deep learning protocols are also employed for generative applications. The idea is to deploy such models to expedite reaction discovery using an ML-guided approach.

Specific research interests:

1. Asymmetric multi-catalytic reactions
 - Asymmetric reactions involving transition metal catalysts and organocatalysts.
 - Origin of enantioselectivity and catalyst design.
2. Mechanistic studies on C-H bond activation reaction
 - Role of additives and solvents
 - Rational modifications to catalysts and substrates
3. Machine learning in catalysis
 - Prediction of reaction outcome
 - Artificial intelligence (AI)-enabled catalyst design

SL13

Theoretical Investigations of Molecular, Supramolecular and Enzyme Catalyzed Organic Transformations: A Density Functional Theory Approach

Lisa Roy^{1,*}

¹ Department of Education, Indian Institute of Technology Kharagpur, Kharagpur 721302, India

Abstract:

Efficient and selective catalysis is predominant in chemistry, enabling the synthesis of molecules and materials with enormous societal and technological impact. Computational chemistry provides a versatile toolbox for studying mechanistic details of catalytic reactions and holds promise to deliver practical strategies to enable the rational *in silico* catalyst design. Diversity in reactivity, nontrivial electronic structure effects, solvation effects and impact of non-covalent weak dispersive interactions introduce additional complexity that represents a pressing challenge to the conventional synthetic methodologies.¹ Modern *in silico* tools such as the density functional theory (DFT) and other sophisticated physical techniques assess the energetic landscape quite accurately and provide critical insights on conformational flexibility in predicting stereo-, regio and chemo-selectivity. Herein, we aim to discuss the factors such as non-covalent interactions (NCIs), steric or confinement effects that leads to fascinating transformations through (organo)metallic, supramolecular, electrochemical and photo-redox catalysis. We discuss how combined effect of NCIs and removal of steric encumbrance underpin chirality in bifunctional squaramide catalysed reactions leading to skeletal diversity in synthesis of azocine derivatives.² We highlight how regioselective and enantioselective transformations are carried out by transition metal catalysts.³ Lastly, we show a supramolecular capsule arrangement of resorcin-arene that facilitates coupling of pyrrole and isocyanates in a solvent-free environment, simply backed by confinement effects.⁴

References:

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- [2] R. Khuntia, S. K. Mahapatra, L. Roy & S. C. Pan, *Chem. Sci.* 14, 10768 (2023)
- [3] N. Navaneetha, S. Maurya, P. Behera, S. B. Jadhav, L. R. Magham, J. B. Nanubolu, L. Roy, R. Chegondi, *Chem. Sci.* **15**, 20379 (2024)
- [4] S. K. Mahapatra, B. Ghosh, L. Roy (in revision).

Bio-Sketch of the Speaker

Prof. Lisa Roy

Department of Education

Indian Institute of Technology, Kharagpur

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Research Career

Ph.D(Science) in Chemistry (awarded in June 2015) from Indian Association for the Cultivation of Science, Kolkata **Postdoctoral Researcher** (July 2015 – October 2017)

Max Planck Institute for Chemical Energy Conversion, Germany Research Group of Prof. Frank Neese; Group leader Prof. Shengfa Ye **DST INSPIRE Faculty Fellow** (October 2017- October 2018) CSIR Central Mechanical Engineering Research Institute, Durgapur **Assistant Professor (Regular)** (November 2018 - August 2024) Institute of Chemical Technology Mumbai - IOC Odisha Campus Bhubaneswar **Assistant Professor Grade I** (since August 2024)

Indian Institute of Technology, Kharagpur

Research Interest

Our primary research interest lies in the broad area of catalysis which include reactivity study of metalloenzyme and model complexes, organo-catalysts, and metal-organic-frameworks/covalent-organic-frameworks to computationally design novel catalytic systems for sustainable energy and resources. We mainly use combined density functional, and wave-function based methods like the multireference and local pair natural orbital coupled cluster techniques and semi-empirical tight binding approaches to deliver a reliable picture of the catalyst active site binding, aggregation, and reaction mechanism. We are mainly focused on three different subtopics:

- Bio-inspired C-H activation or C=C hydroxylation
- Small molecule activation by 3d transition metal
- Non-covalent interaction assisted catalysis

Awards and Recognitions

- DFG funded invitation to the international meeting, BioOxCat, at Bielefeld University, Germany, 2025
- Thieme Chemistry Journals Awardee, 2025
- Jury Member for Chemistry Europe Award Committee (Wiley VcH), 2024
- CSIR ASPIRE Extramural Research Grant, 2024
- Certificate of Excellent Grade in Performance Review Meeting by DST INSPIRE (2023)
- Early Career Advisory Board Member of ChemPhysChem (Chemistry Europe Society, Wiley VcH), since Jan 2023
- SERB POWER (Promoting Opportunities for Women in Exploratory Research) Grant, 2021
- Early Career Advisory Board Member of ChemPlusChem (Chemistry Europe Society, Wiley VcH), since Jan 2021
- Visiting Researcher at the Max Planck Institute for Coal Research, Germany (July 2019)
- DST INSPIRE Faculty Fellowship (2017) in Chemical Sciences Division
- Offered Postdoctoral Fellowship at The Hebrew University of Jerusalem (2017) (not availed)
- Max-Planck Postdoctoral Fellowship July 2015 – Oct 2017
- International Travel Support from SERB in 2012 for participating at the 48th STC held at KIT in Germany

Publications in Journals & Patents - 67

Details of projects handled -5 (as PI); 1 (as co-PI)

SL14

Probing Ligand Effects through Topographic Steric Mapping: Mechanistic Insights from Computational Analysis

Dr. Manoj V. Mane

Centre for Nano and Material Sciences, Jain (Deemed-to-be University),
Jain Global Campus, Bangalore, Karnataka 562112, India

Abstract:

Enantioselective catalysis employs chiral catalysts to preferentially form one enantiomer over the other, offering a powerful approach for the synthesis of high-value molecules. This strategy has transformed modern organic synthesis by enabling sustainable and efficient routes to pharmaceuticals, agrochemicals, and fine chemicals. Computational methods play a pivotal role in identifying and understanding the interactions between ligands and metal centers that govern stereochemical outcomes. Recent computational analyses have deepened our understanding of the structural and energetic factors influencing catalytic selectivity. Tools such as SambVca and NEST provide valuable insights into steric and electronic environments, helping to rationalize and predict enantioselectivity trends. By employing these platforms, one can effectively screen a large library of ligands and prioritize those with superior stereochemical control. In this context, the newly developed chiral-ligands, have demonstrated promising potential in enantioselective catalysis. Tailoring their steric and electronic profiles enhances metal–ligand cooperation and expands their reactivity across diverse catalytic transformations. A key parameter in ligand design, the %V_{Bur}, provides a quantitative measure of steric effects that dictate selectivity in asymmetric reactions. DFT-guided optimization of these ligands facilitates improved substrate accessibility at the catalytic site, leading to enhanced activity and selectivity. A comprehensive mechanistic investigation, supported by DFT calculations, reveals an enantioinduction model governed by the axially chiral C₂-symmetric dihydroazepino-binaphthyl core of the Ad-ChetPhos ligand. Topographic steric maps and %V_{Bur} analyses across key intermediates and transition states elucidate how the ligand's dynamic steric environment drives high enantioselectivity throughout the catalytic cycle.

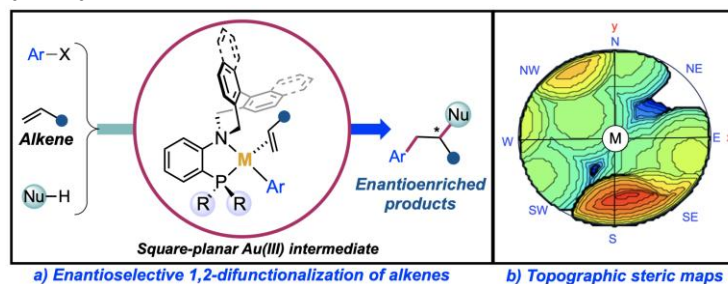


Fig1. Topographic steric maps in catalyst design, (%V_{Bur}) percentage of buried volume.

References:

- [1] L. Falivene, Z. Cao, A. Petta, L. Serra, A. Poater, R. Oliva, V. Scarano, L. Cavallo, *Nat. Chem.* 11, 872–879, (2019).
- [2] G. Zuccarello, *et al J. Am. Chem. Soc. Au* 3, 1742–1754 (2023).
- [3] B. Paroi, C. Chintawar, M. V. Mane, N. T. Patil, *ACS Catal.* 15, 11922-11930, (2025).

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Research Career

Assistant Professor

Research Interest:

Homogeneous Catalysis, Small molecule activation, Dual-Photo catalysis, Ligand design by using computational tools like density functional theory (DFT).

Publications in Journals & Patents

75 Publications

Details of projects handled

ANRF- Prime Minister Early Career Research Grant

SL15

Disorder Engineering in Macromolecular Frameworks for Electrocatalysis Reaction

Dr. Tamas Panda

Center for clean Environment & Dept. of Chemistry, Vellore Institute of Technology, Vellore, 632014

Abstract

Mechanochemical synthesis exhibits enormous potential for the clean, economic, environmental-friendly and efficient route for the structural transformation of molecules and materials. Our recent work based on an attempt to design and synthesis of new phase pure Metal Organic Framework (MOF) materials by solid state hand grinding or ball mill method. Additionally, our research group also focused to do the ball mill induced mechanical engineering on the various MOFs to acquire new type of structures with unique properties. These types of approach are very rare and not attempted earlier in this area of research. We have developed a unique series of pure phase MOFs (ZnTIA-1mc, CuTIA-1mc and CoTIA-1mc) synthesized exclusively by mechanochemical (mc) grinding method (Figure 1). The same synthesis was also attempted in each case by using solvothermal procedure, which result the phase impure mixture of two different MOFs crystals. Kinetics study with the function of grinding time during the mechanosynthesis process revealed that the formation of variety of new metastable phases. Less crystallinity and short of mechanical defects in the structure of synthesized mechanochemical MOFs showed enhanced electrocatalytic activity towards oxygen evolution reaction (OER). In our next work, a novel zeolitic tertrazolate framework (ZTF-8) has been synthesized by green and facile mechanochemical ball mill method with exceptional acid/base stability. The structure of ZTF-8 adopts the zeolitic sodalite (SOD) topology with uncoordinated N-heteroatom sites and resembles with the structure of the well-known zeolitic imidazole framework ZIF-8. Directly used ZTF-8 is the unique report among all the MOFs for the selective electrochemical sensing of dopamine (DA) in the presence of highly concentrated common interferents. Additionally, ZTF-8 electrochemical sensor is the best among all the MOFs in terms of its ability to detect DA in a very wide linear range (5-550 μM) of concentration with excellent sensitivity. DFT study, strongly support our experimental result, revealed that the ZTF-8 framework has a higher binding energy and stronger interaction with dopamine than its isostructural ZIF-8 structure.

References

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3. P. Jhariat, A. Warriar, M.Varghese, Tamas Panda*, *J. Mater. Chem. A*, **2025**, 13, 23893-23901
4. S. Sarfudeen, N. P K, A. Basith, M. Varghese, P. Jhariat, A. Chandrasekhar, Tamas Panda* *ACS Appl. Mater. Interfaces*, **2024**. DOI: 10.1021/acsami.4c00454
5. P. Jhariat, A. Kumar, A. Warriar, A. P. Sunda, S. Das, S. Sarfudeen, V. M. Dhavale, T Tamas Panda*, *ACS Appl. Mater. Interfaces*, **2024**, 16, 18, 23387–2339.
6. S. Sarfudeen, Tamas Panda* *Chem. Eng J.* **2025**, 503, 158519
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8. P. Kumari, A. Kareem, P. Jhariat, S. Senthil, Tamas Panda* *Inorg Chem*, **2023**, 8, 3457-3463.
9. S. Sarfudeen, V. Sruthi, A. maibam, P. Panda, P. Jhariat, S. Senthilkumar, R. Babarao, Tamas Panda* *Inorg Chem*, **2023**, 49, 20236-20241
10. P Jhariat, A Kareem, P Kumari, S Sarfudeen, Tamas Panda* *Dalton Trans*, **2024**, 53, 6568.
11. P. Kumari, Tamas Panda* *Inorg Chem*, **2023**, 38, 15335-15339
12. P. Kumari, Tamas Panda* *Cryst. Growth Des.* **2024**, 24, 11, 4493–4500,
13. P. Jhariat, P. Kumari, Tamas Panda*. *CrystEngComm*. **2020**, 22, 6425-6443.
14. Tamas Panda, S. Horike, K. Hagi, N. Ogiwara, K. Kadota, T. Itakura, M. Tsujimoto, S. Kitagawa, *Angew.Chem., Int. Ed.*, **2017**, 56, 2413.

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Research Career

Dr. Tamas Kumar Panda is an Associate Professor of Chemistry at VIT Vellore, India. He obtained his Ph.D. in Chemistry from CSIR–NCL Pune in 2014 under Prof. Rahul Banerjee, followed by prestigious postdoctoral fellowships at Kyoto University, Japan (2014–2016) under Prof. Susumu Kitagawa (Noble Prize winner 2025), followed by New York University Abu Dhabi (2016–2018) with Prof. Pance Naumov. During his doctoral studies, he was trained in X-ray crystallography and carried out advanced investigations on Metal–Organic Frameworks (MOFs) for selective carbon dioxide and hydrogen storage. His postdoctoral work further advanced the field by introducing a mechanochemical approach for creating solid solutions of MOFs, pioneering an eco-friendly and industrially scalable method for incorporating bifunctionality. At VIT, Dr. Panda leads a research group dedicated to the design and synthesis of porous frameworks such as Metal–Organic Frameworks (MOFs), Covalent Organic Frameworks (COFs), for applications in energy conversion, electrocatalysis, and environmental remediation. His group has demonstrated enhanced triboelectric nanogenerator (TENG) performance using novel nitrogen-rich ZTF-8, developed core–shell MOF nanoarchitectures for humidity sensing, and reported viologen-based ionic COFs as bifunctional electrocatalysts for oxygen reduction, oxygen evolution, and hydroxide conduction. Dr. Panda has authored 40 publications, filed two patents, secured national research funding (SERB, CSIR), and received multiple awards for research excellence. He has delivered invited talks internationally, nationally and actively contributes to academic workshops and conference.

Research Interest

Metal Organic Frameworks, Solid Solutions of MOFs, Covalent Organic Framework, Electrocatalysis, Photocatalysis, Sensing and Separation.

Awards and Recognitions

1. Best Faculty Research award in the year 2021, 2022, 2023 and 2024 at VIT Vellore
2. ACS publication Best Faculty presentation award in the international conference CI3CS-2023 organized by Presidency University, Kolkata.
3. Best presentation award in the international conference ISCBC-2022 held at BIT Mesra at 17th Nov, 2022.
4. JSPS Post-Doctoral Research Fellowship (Japan), September 2014 to August 2016
5. BK21 Post-Doctoral Research Fellowship, South Korea, September 2016 (Offer Declined)
6. Best Poster award in ICMAT13 symposium, Singapore (5th July 2013)
7. Best Research Scholar award at National Chemical Laboratory, Pune (28th Feb, 2013)
8. Best high impact research paper award at National Chemical Laboratory, Pune, (28th Feb, 2014)
9. Best Poster award in National Chemical Laboratory, Pune (28th Feb, 2011).

Publications in Journals & Patents- A total of 40 research papers has been published, including 17 as corresponding author and 23 as first or co-author. In addition, two Indian patents have been published.

Details of projects handled- Successfully completed one DST-SRG project and currently handling a CSIR-EMR-II project.

IL21

Iridium-Catalyzed Enantioselective C–H Allenylation

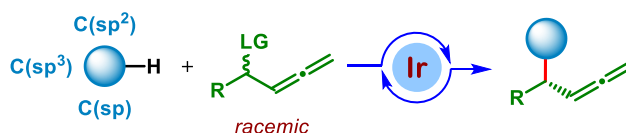
Santanu Mukherjee

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Abstract:

Compared to the widely explored transition metal-catalyzed asymmetric allylic substitution reactions, the corresponding allenyl substitution reactions are much less developed. However, tremendous advancement in this area, especially in the realm of iridium catalysis, took place in the past few years.¹ Our group is interested in unexplored classes of carbon nucleophiles for Ir-catalyzed allenyl substitution reactions, with a special emphasis on C–H allenylation. To this end, we have developed catalytic enantioselective allenyl substitutions with vinyl azides as an amide enolate surrogate² and applied (bis)vinyllogous enol silanes for site-selective allenylation of unsaturated carbonyls.³ We have also developed the first enantioselective Friedel-Crafts allenylation⁴ and enantioselective *meta*-allenylation of pyridines.⁵ Our mechanistic exploration in Ir-catalyzed allenyl substitution led to the discovery of a new mode of cooperative catalysis, namely *divergent cooperative catalysis*, an application of which was demonstrated for the enantioselective homocoupling of allenyl alcohols.⁶ Some of these topics will be covered in this talk.



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- [1] (a) Petrone, D. A.; Isomura, M.; Franzoni, I.; Rössler, S. L.; Carreira, E. M., *J. Am. Chem. Soc.* **2018**, *140*, 4697. (b) Zhang, J.; Huo, X.; Xiao, J.; Zhao, L.; Ma, S.; Zhang, W., *J. Am. Chem. Soc.* **2021**, *143*, 12622.
- [2] Chakrabarty, A.; Mukherjee, S., *Angew. Chem., Int. Ed.* **2022**, *61*, e202115821.
- [3] Mitra, S.; Mukherjee, S., *JACS Au* **2024**, *4*, 4285.
- [4] Das, P.; Ghosh, D.; Mukherjee, S., *Angew. Chem., Int. Ed.* **2024**, *63*, e202413609.
- [5] Roy, P.; Mahto, P.; Mukherjee, S., *Angew. Chem., Int. Ed.* **2025**, *64*, e202511571.
- [6] Chakrabarty, A.; Chatterjee, R.; Mukherjee, S., *Chem. Sci.* **2025**, *16*, 20495.

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Research Career

Professor (since 2021) – at the Department of Organic Chemistry, IISc Bangalore

Associate Professor (2015-21) – at the Department of Organic Chemistry, IISc Bangalore

Assistant Professor (2010-15) – at the Department of Organic Chemistry, IISc Bangalore

Postdoc (2008-10) – with E. J. Corey at Harvard University, Cambridge, MA, USA

Postdoc (2006-08) – with Benjamin List at the Max-Planck Institut für Kohlenforschung, Mülheim, Germany

PhD (2006) - Universität zu Köln, Germany

Research Interest

Asymmetric Catalysis (Organocatalysis, Transition Metal Catalysis, Cooperative Catalysis),
Stereoselective Synthesis, Natural Product Synthesis

Awards and Recognitions

- Associate Editor, *Chemical Communications* (since 2025)
- *SYNLETT* Best Paper Award 2023
- SERB-STAR Award (2021)
- AV Rama Rao (AVRA) Young Scientist Award for the year 2019
- Chemical Research Society of India (CRSI) Bronze Medal (2021)
- Associate Editor, *Organic & Biomolecular Chemistry* (since 2019)
- Indian National Science Academy (INSA) Medal for Young Scientist (2014)
- Thieme Chemistry Journals Award (2011)

IL22

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

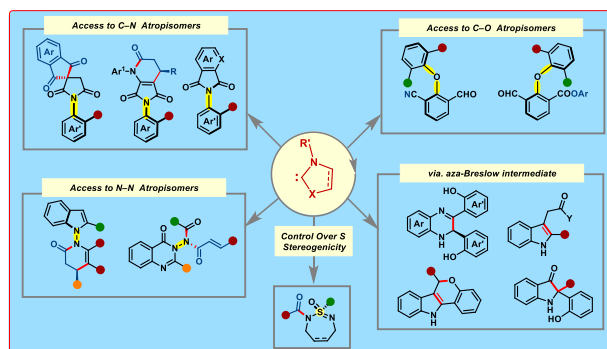
Akkattu T. Biju

Department of Organic Chemistry, Indian Institute of Science, Bangalore-560012, India

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Abstract:

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 been achieved by the enantioselective synthesis of N-acyl cyclic sulfonimidamides.⁶ The details of these works will be discussed.



References

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- Barik, S.; Shee, S.; Das, S.; Gonnade, R. G.; Jindal, G.; Mukherjee, S.; Biju, A. T. *Angew. Chem. Int. Ed.* **2021**, *60*, 12264.
- Barik, S.; Ranganathappa, S. S.; Biju, A. T. *Nat. Commun.* **2024**, *15*, 5755.
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- (a) Shee, S.; Ranganathappa, S. S.; Gadhave, M. S.; Gogoi, R.; Biju, A. T. *Angew. Chem. Int. Ed.* **2023**, *62*, e202311709. (b) Shee, S.; Ramachandran, D.; Gogoi, R.; Biju, A. T. *ACS Catal.* **2025**, *15*, 13157.

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Advisory Board, *Org. Chem. Front.*

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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.

IL23

Asymmetric N-Heterocyclic Carbene Catalysis via Noncovalent Interaction

Joyram Guin

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Abstract:

N-heterocyclic carbenes (NHCs) play a crucial role in asymmetric organocatalysis. They can activate substrates through either covalent or non-covalent interactions (Figure 1), which presents a unique opportunity to develop a variety of asymmetric transformations using numerous substrates. Indeed, many impressive asymmetric transformations have been accomplished through NHC catalysis, particularly via covalent interactions with substrates that contain activated carbonyl functional groups. In contrast, noncovalent NHC catalysis, while significantly broadening the scope of NHC applications, is still in its early stages of development.¹ Our research group is actively engaged in developing new enantioselective organic transformations utilizing the noncovalent mode of NHC catalysis. Some recent findings² from our group in this area will be discussed during the lecture.

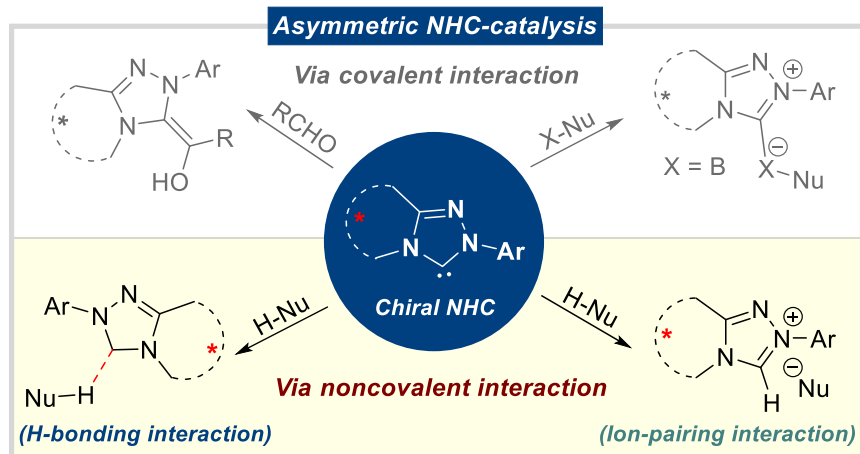


Figure 1: Different modes of asymmetric NHC-catalysis

References:

- (a) E. Li, X. Liao, F. Guo, Y. Huang and J. Chen, *Org. Lett.*, 2024, **26**, 7479-7483; (b) E. Li, Q. Wang, Y. Cai, J. Chen and Y. Huang, *Cell. Rep. Phys. Sci.*, 2021, **2**, 100490; (c) P. Yuan, S. Meng, J. Chen and Y. Huang, *Synlett*, 2016, **27**, 1068-1072; (d) J. Chen and Y. Huang, *Nat. Commun.*, 2014, **5**, 3437.
- (a) U. Maji, A. Baidya, S. Das and J. Guin, *Org. Lett.*, 2025, **27**, 2423-2428; (b) B. D. Mondal, S. Gorai, R. Nath, A. Paul and J. Guin, *Chem. Eur. J.*, 2024, **30**, e202303115; (c) U. Maji, S. Das, A. Baidya, I. Roy and J. Guin, *Org. Lett.*, 2024, **26**, 8719-8724; (d) U. Maji, B. D. Mondal and J.

Guin, *Org. Lett.*, 2023, **25**, 2323-2327; (e) S. Santra, U. Maji and J. Guin, *Org. Lett.*, 2020, **22**, 468-473; (f) S. Santra, A. Porey, B. Jana and J. Guin, *Chem. Sci.*, 2018, **9**, 6446-6450.

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Research Career

- Professor (since January 2021): School of Chemical Sciences, IACS, India
- Associate Professor (2017-2020): School of Chemical Sciences, IACS, India
- Assistant Professor (2013-2016): Department of Organic Chemistry, IACS, India
- Postdoctoral Fellow (2010-2012): Max-Planck-Institut für Kohlenforschung, Germany (*Advisor: Professor Benjamin List, Nobel laureate 2021*)
- Postdoctoral Fellow (2008-2010): University of Geneva, Switzerland (*Advisor: Professor Jerome Lacour*)
- Ph.D. (2004-2007): International Graduate School of Chemistry, Westfälische Wilhelms-Universität, Muenster, Germany (*Advisor: Professor Armido Studer*)

Research Interest

- Free-radical mediated C-H functionalization using O₂ as a green oxidant
- Asymmetric organocatalysis using N-heterocyclic carbenes (NHCs)
- Organic synthesis involving photocatalysis and HAT catalysis
- Pd-catalyzed oxidative C-H functionalization
- Olefin difunctionalization using dual Ni/photoredox catalysis

IL24

Leveraging Non-classical σ -hole based Noncovalent Interactions and Asymmetric Catalysis: Emerging Frontiers in Stereoselective Carbohydrate Synthesis

Charles C. J. Loh^{1*}

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Abstract:

There is a recent renaissance amongst organic chemists in appreciating the value of stereoselective carbohydrate synthesis as an excellent platform for discovery of chemical phenomena.^[1] In my talk, I will describe two emerging directions pursued by my research group. In the first direction, I will narrate our seminal efforts in developing mild and robust σ -hole based noncovalent catalyzed methods for selective carbohydrate synthesis – an approach we now define as the “ σ -hole based catalytic glycosylation strategy”.^[2-3]

I will offer an overview of our early efforts in the development of exclusively halogen bonding (XB) catalyzed strain-release glycosylation and 2-deoxyglycosylation. These strategies contain unique advantages, such as the elevation of anomeric selectivity. Next, I will introduce our pioneering approach in chalcogen bonding (ChB) catalyzed glycosylations and glycomimetic synthesis. We recently demonstrated that the ChB catalysis performed exceptionally well on glycosyl substrates. We further developed versatile strategies that enabled access into biologically relevant 7-membered ring sugars known as septanosides,^[4] β -indolyl glycosides^[5] as well as in underexplored iminoglycosides.^[6] A second research axis is the harnessing of metal catalyzed asymmetric catalysis to surmount multiple enantio-, diastereo- and site-selectivity challenges within a single bond forming step.^[2] Besides sharing novel asymmetric rhodium^[7] and radical copper catalyzed^[8] platforms we developed, I will touch on recent efforts to exploit NCIs for carbohydrate stereocontrol in the context of asymmetric palladium catalyzed site-selective functionalizations.^[9]

Research:

[1] C. C. J. Loh, *Angew. Chem. Int. Ed.* 64, e202514167 (2025).

[2] A. T. Sebastian, C. C. J. Loh, *Acc. Chem. Res.* 58, 2124-2144 (2025).

[3] C. C. J. Loh, *Nat. Rev. Chem.* 5, 792-815 (2021).

[4] W. Ma, J.-L. Kirchhoff, C. Strohmman, B. Grabe, C. C. J. Loh, *J. Am. Chem. Soc.* 145, 26611-26622 (2023).

[5] H. Guo, J.-L. Kirchhoff, C. Strohmman, B. Grabe, C. C. J. Loh, *Angew. Chem. Int. Ed.* 63, e202316667 (2024).

[6] C. Wang, A. Krupp, C. Strohmman, B. Grabe, C. C. J. Loh, *J. Am. Chem. Soc.* 146, 10608-10620 (2024).

[7] V. U. Bhaskara Rao, C. Wang, D. P. Demarque, C. Grassin, F. Otte, C. Merten, C. Strohmman, C. C. J. Loh, *Nat. Chem.* 15, 424-435 (2023).

[8] H. Guo, D. Tan, C. Merten, C. C. J. Loh, *Angew. Chem. Int. Ed.* 63, e202409530 (2024).

[9] H. Guo, J.-L. Kirchhoff, C. Strohmman, B. Grabe, C. C. J. Loh, *Angew. Chem. Int. Ed.* 63, e202400912 (2024).

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Research Career

- 2016-2024 **Research Group leader**,
Max Planck Institute für molekulare Physiologie, Dortmund, Germany
- 2014-2016 **Postdoctoral researcher**, University of Toronto, Canada
Advisor: Prof. Dr. Mark Lautens
- PhD studies**, Institute of Organic Chemistry, RWTH Aachen University,
Germany.
2010-2013 Supervisor: Prof. Dieter Enders

Research Interest

Development of non-classical σ -hole based glycosylation methods and asymmetric catalytic strategies for site-selective carbohydrate functionalizations using a mechanistically driven approach.

Awards and Recognition

- 2025 Advanced Science Young Innovator Award (Wiley)
- 2021-2024 Plus 3 Perspectives Programme of the Boehringer Foundation
- 2016-2021 Liebig fellowship of the Fonds der Chemischen Industrie
- 2014-2016 German research foundation (DFG) post-doctoral fellowship
- 2014 Borschers Plakatte, RWTH Aachen University (*summa cum laude*)

Publications in Journals & Patents

33

Details of projects handled

4

Technology development/ Initiation

Pioneering the σ -hole based catalytic glycosylation strategy.

OL5

Supramolecular Materials with Tunable Properties for Advanced Aqueous Separations

Shilpi Kushwaha

CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar, India.

shilpik@csmcri.res.in; shilpi.kushwaha@fulbrightmail.org

Abstract:

Supramolecular self-assembled materials driven by non-covalent secondary interactions present a powerful platform for engineering functional frameworks with tunable molecular architecture and stability. Their intrinsic advantages—ease of synthesis, processability, flexibility, hydrolytic stability, and reversible self-healing—make them attractive for large-scale aqueous separation technologies. Achieving angstrom-level control over porosity remains a central challenge in translating molecular design into selective separation media. Through rational molecular engineering and linker selection, supramolecular assemblies can now be organized into crystalline frameworks exhibiting well-defined intrinsic pores and tunable extrinsic porosity, enabling precise molecular discrimination across large areas. These features, coupled with exceptional hydrolytic and mechanical robustness, make them ideal for applications such as selective molecular and ionic separations, uranium extraction from seawater, and catalytic oxygen evolution in saline environments. The development of these advanced materials is guided by targeted design parameters: (i) long-range structural order, (ii) high permeability and selectivity, (iii) interconnected porosity, (iv) mechanical, hydrolytic, and chemical stability, (v) corrosion resistance, and (vi) processability, regenerability, and scalability.

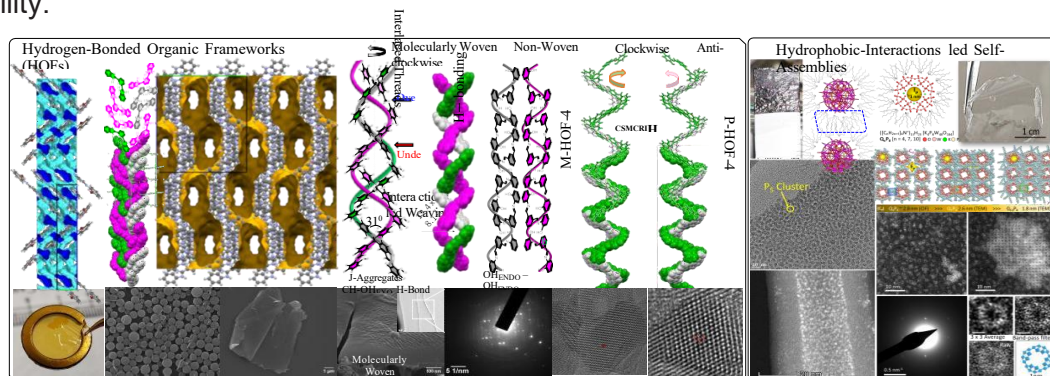


Figure 1. Supramolecular Materials

References:

- Sholl, D. S.; Lively, R. P. *Nature* 2016, 532, 435; Abney, C.W.; Mayes, R.T.; Saito, T.; Dai, S. *Chem. Rev.* 2017, 117, 13935; Kanan, M.W. & Nocera, D. G. *Science* 2008, 321, 1072; Poblet J.M. et. al, *JACS* 2007, 129, 12244
- Kushwaha et al. *Trends in Chemistry*, 2025, 7(9), 490-493. *Small* 2024, 20, 2310797. *Small* 2024, 20, 2306824. *ACS Catalysis* 2023 13, 4587-4596. *Chem* 2022, 8, 2749-2765 (**Highlighted in ACS C&EN 2022, 100, 29.**) *Chem* 2021, 7(2), 1-4.

Bio-Sketch of the Speaker

Dr. Shilpi Kushwaha

Sr. Scientist

CSIR-Central Salt & Marine Chemicals Research Institute

shilpi@csmcric.res.in



Research Career:

Ph.D. Chemistry (2012), M.Sc. Applied Chemistry (2007), B.Sc. Chemistry (2005), Fulbright-Nehru Post-Doctoral Scholar (2013-14), DST-Young Scientist (2015-18)

Research interests:

1. **Material Design** (Supramolecular self-assemblies, Woven materials, HOFs, Polymers, Porous Carbons, nano-dots etc...);
2. **Post-Modification of Materials** (Functionalization of Polymers, HOFs, Supramolecules, Carbons etc...);
3. **Nano-materials** (Downsizing the bulk-synthesized materials);
4. **Spectroscopic Techniques, Thermodynamic & Analytical Modelling** for deriving mechanisms;
5. **Surface Chemistry** (Liquid-liquid/ Air-Liquid/ Solid-Air/ Solid-Liquid);
6. **Separation Science** (Adsorptive/ Size-exclusion/ Diffusion-based etc...);

Awards:

1. CSIR Young Scientist Award for the year 2021 in Earth, Atmosphere, Ocean and Planetary Sciences for the innovative research on the extraction of Uranium from secondary sources such as seawater and acidic effluents using crystalline thin films and polymer nanorings, September 2021.
2. 1st Prize for Oral presentation in National Conference on Recent Trends in Science of Materials (NCSM-2015).
3. OLF Award from CIES, USA (2014).
4. Fulbright Post-Doctoral Fellowship (2013-14).
5. Senior Research Fellow BRNS (2009-10)
6. DST international travel grant (2008)
7. Indian National Science Academy support for hospitality (2008)
8. Junior Research Fellow BRNS (2007- 2009)

OL6

Repurposing Metal-Acylnitrenoids Reactivity: A Formal Remote C–H Functionalization of Carboxylic Acids

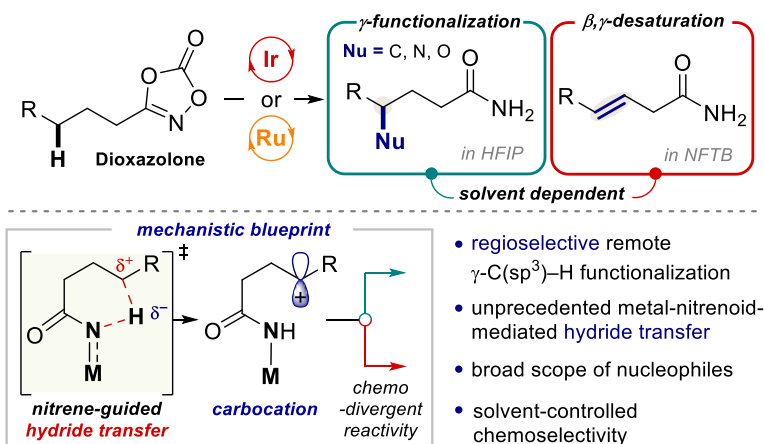
Sourav Pradhan,¹ Jeonguk Kweon, Manoj Kumar Sahoo, Hoimin Jung, Joon Heo, Yeong Bum Kim, Dongwook Kim, Jung-Woo Park,* and Sukbok Chang*²

¹Mahindra University, Hyderabad, India.

²Institute for Basic Science, Korea Advanced Institute of Science and Technology, Daejeon South Korea.

Abstract:

Harnessing the key intermediates in metal-catalyzed reactions is one of the most essential strategies in the development of selective organic transformations. The nitrogen group transfer reactivity of metal-nitrenoids to ubiquitous C–H bonds allows for diverse C–N bond formation to furnish synthetically valuable aminated products. In this study, we present an unprecedented reactivity of iridium and ruthenium nitrenoids to generate remote carbocation intermediates, which subsequently undergo nucleophile incorporation, thus developing a formal γ -C–H functionalization of carboxylic acids. Mechanistic investigations elucidated a unique singlet metal-nitrenoid reactivity to initiate γ -hydride abstraction to form the carbocation intermediate that eventually reacts with a broad range of carbon, nitrogen, and oxygen nucleophiles, as well as biorelevant molecules. Alternatively, the same intermediate can lead to deprotonation to afford β,γ -unsaturated amides in a less nucleophilic solvent.



References:

- [1] S. Pradhan, J. Kweon, M. K. Sahoo, H. Jung, J. Heo, Y. B. Kim, D. Kim, J.-W. Park, S. Chang *J. Am. Chem. Soc.* 145, 28251 (2023).
- [2] Y. Hong, Y. Hwang, M. Lee, S. Chang *Acc. Chem. Res.* 54, 2683 (2021).

CONTACT/PRESENTING AUTHOR

*Sourav Pradhan; sourav.pradhan@mahindrauniversity.edu.in

Bio-Sketch of the Speaker

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Mahindra University, Hyderabad, India
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Research Career

Dr. Pradhan is currently an Assistant Professor in the Department of Chemistry at École Centrale School of Engineering, Mahindra University, Hyderabad. His research focuses on the development of novel organic fluorophores using C-H functionalization, bioconjugation, target oriented synthesis using photoredox catalysis and method development towards sustainable and green chemistry applications.

- Ph.D. (2014–2020): Indian Institute of Technology Guwahati, Assam, India
- M. SC. (2011–2013): Indian Institute of Technology Bombay, Powai, India
- B. Sc. (2008–2011): Vidyasagar University, West Bengal, India
- **Assistant Professor** (2025–present): Mahindra University, Hyderabad, India
- **Senior Researcher** (2023–2025): Institute for Basic Science, Korea Advanced Institute of Science and Technology, South Korea
- **Postdoctoral Research Associate** (2021–2023): Institute for Basic Science, Korea Advanced Institute of Science and Technology, South Korea
- **Research Associate** (10/2020–03/2021): Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, Karnataka

Research Interest

- Co-operative Catalysis
- Photoredox Catalysis and Bioconjugation
- Organic Fluorophores

Day 2 – 18-11-2025, Auditorium 2

IL18

**Development of Catalysts for Achieving a Sustainable Society:
Examples from the Chemical Industry and Energy Technologies**

Matthias Beller¹

¹ Leibniz-Institut für Katalyse, Albert-Einstein-Str. 29a, 18059 Rostock, Germany.
matthias.beller@catalysis.de

Abstract:

The use of renewables, waste, and carbon dioxide for the cost-effective and waste-free synthesis of materials, life science goods and all kinds of organic products can be an important part to achieve a circular economy in the future. In this respect, efficient catalytic reductive transformations of CO₂ offer interesting possibilities to replace existing industrial carbonylations. Nowadays, in the chemical industry, carbonylation processes constitute the largest applications of homogeneous catalysts and many bulk and fine chemicals are produced by such transformations.

In the talk, various possibilities to use green CO from CO₂/H₂ mixtures, formic acid as CO surrogate or directly CO₂ will be shown. Crucial for all these reactions is the development of modern catalysts. By rational design novel ligands and complexes have been synthesized, which allow for unprecedented efficiency in such transformations. Both industrially relevant processes as well as interesting carbonylation reactions for modern organic synthesis will be presented. Furthermore, it will be shown how carbon dioxide itself can contribute to realize CO₂-neutral energy technologies.

Bio-Sketch of the Speaker

Prof. Matthias Beller

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Director of the Leibniz Institute for Catalysis at the University of Rostock (Germany)

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Education:

- 1987 Undergraduate degree, University of Göttingen (Germany)
- 1989 PhD with L.-F. Tietze, University of Göttingen
- 1990 Liebig Scholar with K. B. Sharpless, Massachusetts Institute of Technology

Awards:

- 2003 Novartis Chemistry Lecturer; 2006 Gottfried Wilhelm Leibniz Prize of the DFG; Cross of
- the Order of Merit of the Federal Republic of Germany; 2010 Paul Rylander Award of the
- Organic Reactions Catalysis Society (USA); 2011 European Sustainable Chemistry Award,
- American Chemical Society GCI Pharmaceutical Roundtable Lecturer; 2012 Prix Gay-Lussac
- Humboldt

Current research interests:

Development of new sustainable catalysts for practical applications, namely coupling and carbonylation reactions, selective redox processes, development of iron catalysts, and the application of catalysis to more benign energy technologies

IL19

Saturated *N/O*-heterocycles for medchem

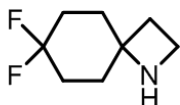
Pavel K. Mykhailiuk

Enamine Ltd. Chervonotkatska 78, 02094 Kyiv (Ukraine).

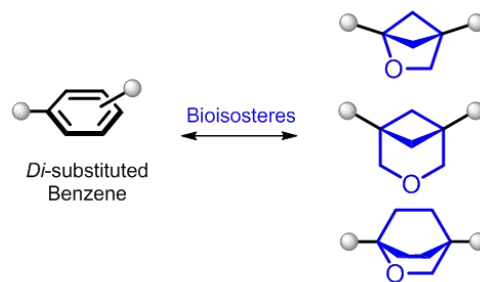
Email: Pavel.Mykhailiuk@gmail.com

Recent advances in the synthesis of saturated *N/O*-heterocycles, and their application in medchem will be provided [1].

Saturated *N*-heterocycles



Saturated *O*-heterocycles



European Research Council

Established by the European Commission

References:

<https://mykhailiukchem.org/2024-2025>

Bio-Sketch of the Speaker

Pavel Mykhailiuk, PhD

Enamine Ltd.

Pavel was born in Kerch, Ukraine. In 2009 he received PhD in biochemistry from Technical University of Karlsruhe (KIT, Germany) with Prof. Anne Ulrich; and PhD in organic Chemistry from Kyiv National Taras Shevchenko University (Ukraine) with Prof. Igor Komarov.



In 2009, Pavel returned to Ukraine and joined “Enamine” company, where he is currently involved into discovery of novel building blocks for drug design.

Pavel’s research interests include fluoroorganic chemistry, chemistry of diazo compounds, photochemistry and saturated bioisosteres of the benzene. He is co-author of more than 100 peer-reviewed research manuscripts. In 2017, he received Dr.Sci. in organic chemistry from the Kyiv National Taras Shevchenko University.

Research Career

2017

Dr. Sci. in organic chemistry with Prof. A. Tolmachev
National Taras Shevchenko University of Kyiv (Ukraine).

2005-09

PhD in biochemistry with Prof. A. Ulrich
Karlsruhe Institute of Technology (Germany).

2005-09

PhD in organic chemistry with Prof. I. Komarov
National Taras Shevchenko University of Kyiv (Ukraine)

Grants and Awards

2024Liebig Lecturer 2024.

2021RSC Fluorine Award for 2021 (under 40).

2020ERC consolidator grant ERC consolidator grant (ID: 101000893).

2018Finalist of “The European Young Chemist Award” (12 European chemists under 35).

2017“Prize of the President of Ukraine for young scientists” (under 40).

2016Finalist of “The European Young Chemist Award” (13 European chemists under 35).

2016“Ukrainian Scopus Award” (under 35).

2015“Prize of National Academy of Science (NAS) of Ukraine” (under 35).

2014Runner-up of EFMC Prize for a Young Medicinal Chemist in Industry (under 35).

2008“Wolff & Sohn-Prize” at Karlsruhe Institute of Technology, (Karlsruhe, Germany).

2000Bronze medal at “32nd International Chemistry Olympiad” (Copenhagen, Denmark).

1999Silver medal at “33d Mendeleev Chemistry Olympiad” (Minsk, Belarus).

Research Visits

IL20

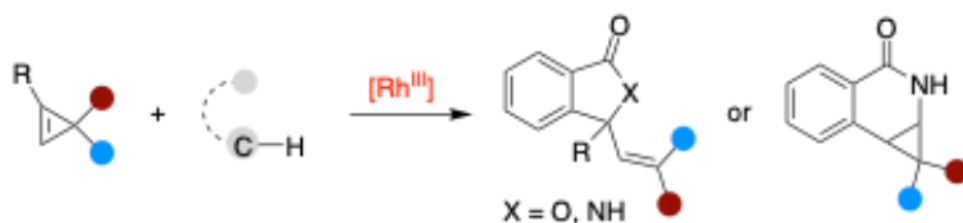
Ligand Controlled Chemo- and Stereodivergent Functionalization of C-H bonds with Cyclopropenes

Pazhamalai Anbarasan

Department of Chemistry, Indian Institute of Technology Madras, Chennai – 600036

Abstract:

Metallocarbenes show versatile reactivity in organic synthesis and offers access to diverse complex frameworks in single step. Most often these metallocarbenes are generated from reactive α -diazocarbonyl compounds in the presence of suitable transition metal.^[1] In the quest of finding suitable alternative, cyclopropenes have emerged as unique surrogates and offers structurally different metallocarbenes, viz. metallovinylcarbenes, which possess distinct reactivity.^[2] The unique reactivity of these metallocarbene precursor have been efficiently integrated with the C-H bond functionalizations for the multisubstituted allylation of arenes and enantiodivergent annulation reactions.^[3] In this presentation, our efforts on the catalytic functionalization of C-H bonds with cyclopropenes and their asymmetric version will be discussed.



References:

- [1] a) Doyle, M. P. *Chem. Rev.* **1986**, 86, 919; b) Davies, H. M. L.; Moron, D. *Chem. Soc. Rev.* **2011**, 40, 1857.
- [2] a) Zhang, H.; Wang, B.; Yi, H.; Zhang, Y.; Wang, J. *Org. Lett.* **2015**, 17, 3322; b) González, M. J.; González, J.; López, L. A.; Vicente, R. *Angew. Chem., Int. Ed.* **2015**, 54, 12139; c) Ross, R. J.; Jeyaseelan, R.; Lautens, M. *Org. Lett.* **2020**, 22, 4838.
- [3] a) Ramachandran, K.; Anbarasan, P. *Chem. Sci.* **2021**, 12, 13442; b) Bakkiyaraj, M.; Anbarasan, P. *Org. Lett.* **2025**, 27, 1638; c) Bakkiyaraj, M.; Adak, P.; Anbarasan, P. *ACS Catal.* **2025**, 15, 15808. d) Bakkiyaraj, M.; Anbarasan, P. *manuscript under preparation*.

Bio-Sketch of the Speaker

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Department of Chemistry, IIT Madras

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Homepage: <https://home.iitm.ac.in/anbarasansp/>



Research Career

Anbarasan obtained PhD on the enantioselective total synthesis of natural product from Indian Institute of Science, Bangalore with Prof. Kavirayani R. Prasad, in 2007. Subsequently, he held postdoctoral position at Leibniz Institute for Catalysis, Germany as Alexander von Humboldt fellow with Prof. Matthias Beller and University of California, Berkeley, USA with Prof. Dean Toste. He joined the Department of Chemistry, Indian Institute of Technology Madras (IITM) in Dec-2011, where currently he is a Professor of Chemistry.

Research Interest:

- Design and development of asymmetric transformations
- Stereoselective functionalization of metallocarbenes
- Trifluoromethylation and trifluoromethylthiolation
- Synthesis of therapeutically important natural products

Awards and Recognitions:

AVRA Young Scientist Award, 2021 – SwarnaJayanti Fellowship, 2019-20 – CRSI-Bronze Medal, 2020 – Young Scientist Award of the Academy of Sciences, Chennai, 2020 – CRSI-Young Scientist Award, 2019 – ISCB Young Scientist Award, 2017 – NASI-Young Scientist Platinum Jubilee Award, 2016 – Institute Research & Development Award (IRDA) of IIT Madras, 2015-2016 – Young Scientist Medal of the Indian National Science Academy (INSA), 2015 – Associate Member of the Indian Academy of Sciences, Bangalore (2015-2018) – DAE-Young Scientist Research Award – Thieme Chemistry Journals Award-2013 – Alexander-von-Humboldt fellowship

No. of publications: 104

No. of patents: 4

No. of book: 1

No. pf projects handled: 8

IL25

Effect of particle size on the activity of palladium catalysts

Narayana Kalevaru*, Sebastian Wohlrab

Leibniz Institute for Catalysis (LIKAT), Albert-Einstein-Str. 29a, 18059 Rostock, Germany

Abstract:

Pd-based catalysts are extensively used for a variety of catalytic reactions in general and acetoxylation in particular [1,2]. Acetoxylation of simple olefins like ethylene to vinyl acetate and propylene to allyl acetate are known commercial processes. However, the extension of this work from simple olefins to aromatics is still under developmental stage. As a model reaction, we explored the acetoxylation of toluene to benzyl acetate (BA) using Pd catalysts as an attractive approach for producing benzyl acetate in one step in a gas phase continuous process. In this contribution, we discuss the effects of different solid-state properties of Pd catalysts on the activity, selectivity and long-term stability. The aim of this study is to understand the deactivation phenomenon, reduce the induction period and gain deeper insights on the changes being occurred in Pd size, surface composition, and distribution of different Pd species on the surface of the catalysts at different stages of the reaction.

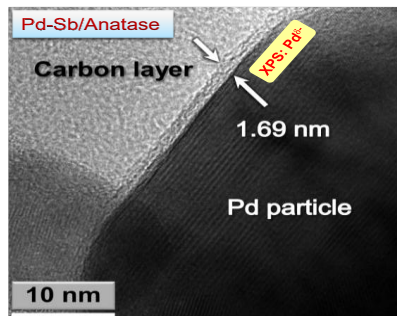
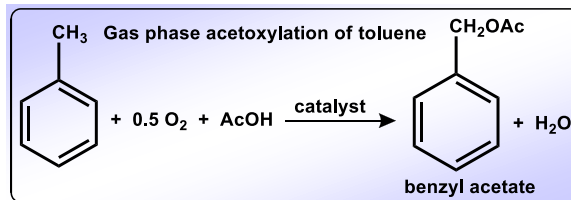


Fig. 1. TEM of deactivated Pd

Results showed that the Pd particle size, nature of support, surface composition played a dominant role on the catalytic performance. TEM analysis of maximum active catalyst (Pd-Sb/TiO₂) revealed the formation of Pd particles of desired Pd size (50-100 nm) with a uniform composition of Pd and Sb (i.e. Pd/Sb=5) that is required for better performance. XPS indicates that fresh catalyst contains mainly PdO_x species on the surface, maximum active solid (after 11h) contains both Pd and PdO_x while the deactivated sample (after 32h) contains both Pd and Pd⁰ species. This result suggests that PdO_x species undergo gradual reduction during the course of the reaction.

The surface composition of the catalysts also exhibits strong influence on the reducibility of Pd species. The coke deposition which in turn leads to the formation of Pd⁰ species is the main cause of catalyst deactivation (Fig. 1). The formation of Pd⁰ species is expected from the interaction between surface Pd atoms and surface carbon-species from coke deposits.

Results revealed strong evidence that the presence of both metallic and oxidised Pd species is necessary for improved activity, selectivity and long-term stability. The palladium catalyst surface is very dynamic and undergoes restructuring during the course of the reaction. Changes in surface composition and formation of Pd⁰ species leads to the deactivation of the catalysts.

References

1. J. Radnik, A. Benhmid, V.N. Kalevaru, M.-M. Pohl, A. Martin, B. Lücke, U. Dingerdissen, *Angew. Chem. Int. Ed.* 44, 6771 (2005).
2. a) N. Madaan, S. Gatla, V.N. Kalevaru, J. Radnik, B. Lücke, A. Brückner, A. Martin, *J. Catal.* 282, 103 (2011); b) S. Reining, E.V. Kondratenko, V.N. Kalevaru, A. Martin, *ACS Catal.* 6, 4621 (2016).

Bio-Sketch of the Speaker

Dr. Narayana V. Kalevaru

Leibniz Institute for Catalysis (LIKAT)

Albert-Einstein-Str. 29a, 18059 Rostock, Germany

Phone No.: +49-381-1281 284

E-mail: narayana.kalevaru@catalysis.de



Research Career

Completed Master's degree (M.Sc.) in Chemistry from Kakatiya University, India and PhD from Indian Institute of Chemical Technology (IICT), Hyderabad.

After PhD, moved to Germany in April 2000. He has been working as a scientist at LIKAT for the past 25 years. Handling various heterogeneous catalytic reactions under gas phase conditions using fixed bed reactors. Guiding PhD students, working with German and European chemical industries on various projects etc.

Research Interests

Heterogeneous Catalysis, Selective oxidations and ammoxidations, Catalyst syntheses and Characterisation, Fixed bed reactors, Gas phase reactions, Natural gas & CO₂ utilisation, Oxy-chlorination of ethylene to vinyl chloride, Oxidative coupling of methane to light olefins, Depolymerisation of plastics, Biomass valorisation and so on.

Publications in Journals & Patents

Publications: ca. 130

Patents: >35

Details of projects handled >25

Industrially important projects handled: i) one-step synthesis of vinyl chloride from ethylene oxy-chlorination ii) Conversion of natural gas and biogas to useful chemicals (i.e. oxygenates, e.g. HCHO), iii) CO₂ utilisation (e.g. conversion of ethylene to acrylic acid using CO₂), iv) oxidative dehydrogenation of light alkanes to olefins, v) Ammoxidation of various aromatic and heteroaromatic hydrocarbons to valuable nitriles and so on. All reactions were carried out in gas phase using various heterogeneous catalysts in fixed bed reactors. Team leader for various other projects like i) Direct synthesis of dimethylcarbonate (DMC) from methanol and CO₂ under supercritical conditions, ii) Synthesis of DMC from urea, iii) One step synthesis of diethylcarbonate (DEC) from ethanol and CO₂, iv) Methyl chloride coupling to light olefins, v) Oxidative coupling of methane to light olefins etc. Other projects: i) Direct hydroxylation of benzene to phenol, ii) Novel process for oxidative methylation of toluene with methane to styrene and ethyl benzene, iii) Simultaneous coupling of dehydrogenation and hydrogenation reactions in one step, iv) Partial oxidation of methane and bio-gas to formaldehyde, v) In-depth studies (e.g. transient isotopic studies) on gas phase acetoxylation of toluene to benzyl acetate using TAP reactor and SSITKA (in-house project), vi) Bio-mass valorisation (e.g. conversion of γ -valerolactone to methyl pentenoates), vii) Valorisation of bio-refinery side streams to building blocks, viii) Nitro reductions at ambient T & P, reductive aminations, dimethylations in liquid phase, ix) Direct synthesis of pure HI from elementary reaction of H₂ and I₂ under gas phase continuous process etc.

SL16

Photo-Triggered Synthesis of Heterocyclic Compounds Via C-S and C-N Bond Formation

Sundaram Singh

Department of Chemistry, IIT(BHU), Varanasi-221005

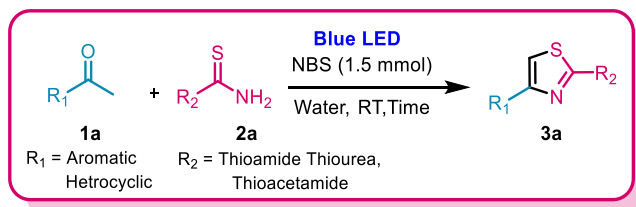
sundaram.apc@itbhu.ac.in

Abstract:

In organic synthesis, photocatalyst-initiated organic transformations are increasingly powerful tools for forming new chemical bonds due to enhanced environmental sustainability and more friendly operating conditions.¹⁻³ One of the primary objectives of modern synthetic chemistry is to develop kinder, more environmentally friendly methods for developing various heterocyclic compounds via C-N and C-S bond formation in place of antiquated, harsher protocols. Generally speaking, these more modern methods are less damaging and easier to use. In general, these more recent techniques are easier to handle and less harmful. On the other hand, photocatalysts based on transition metals such as polypyridyl complexes, ruthenium, and iridium have a number of disadvantages, such as high cost, low sustainability, possible toxicity, and separation challenges.⁴⁻⁷ Numerous studies on the photochemistry of eosin Y under visible light have shown that it quickly crosses between systems to reach the lowest energy triplet state⁸. Metal-free organic dyes, such as eosin Y, are favoured over metal-based photo-redox catalysts because they are more affordable and environmentally friendly.⁹ For important chemical reactions, visible light-mediated photo-redox catalysis for single electron transfer (SET) has recently come to be recognised as a flexible, cost-effective, and environmentally benign method. As a continuous work in the field of green synthetic chemistry, wherein we would like to report a facile, metal-free, and visible light-mediated approach for the development of heterocyclic compounds via C-N and C-S bond formation using a photocatalyst (Scheme 1 and 2).



Scheme1



Scheme2

Reference:

- [1]. Kudo, A.; Miseki, Y., *Chem. Soc. Rev.* **2009**, 38, 253-278.
- [2]. Xuan, J.; Xiao, W. J., *Angew. Chem. Int. Ed.* **2012**, 51, 6828-6838.
- [3]. Schultz, D. M.; Yoon, T. P., *Sci.* **2014**, 343, 1239176.
- [4] Tambe, S. D.; Rohokale, R. S.; Kshirsagar, U. A., *Eur. J. Org. Chem.* **2018**, 2018, 2117-2121.

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Prof. Sundaram Singh

Professor

Department of Chemistry,

Indian Institute of Technology (BHU), Varanasi – 221 005, India

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Research Interest

Synthetic Organic Chemistry, Microwave Assisted Organic Synthesis, Multi-Component Synthesis



SL17

Harnessing the Versatile Reactivity of α -Aminonitriles: A Pathway to Value-Added Molecules

Gopal Chandru Senadi^{1*}, Swetha Sathyendran¹, Vikraman Ganesh Moorthi¹

¹ Green and Sustainable Synthesis Laboratory, Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Chennai, Tamil Nadu, India.

Abstract:

α -Aminonitrile derivatives have emerged as versatile synthetic linchpins owing to their unique bifunctional reactivity. The intrinsic ambiphilicity of α -aminonitriles enables divergent transformations under distinct activation modes, allowing access to structurally diverse and valuable molecular scaffolds. This talk highlights the multifaceted reactivity of α -aminonitriles under Lewis acid and Brønsted base catalysis, showcasing their potential as unified precursors for the construction of amides, imides, quinolines, and imidazoles.

Under Brønsted basic conditions, α -aminonitriles exhibit umpolung reactivity, wherein the inherent polarity of the nitrile carbon is reversed, enabling activation toward oxidative decyanation in the presence of molecular oxygen. This transformation furnishes amide and imide derivatives through a base-promoted oxidation process involving transient carbanion intermediates. In contrast, Lewis acid activation triggers the in-situ formation of an iminium ion from the α -aminonitrile, which subsequently undergoes a formal [4+2] annulation with terminal alkynes or alkenes to afford diverse nitrogen-containing heterocycles. Remarkably, when *N*-acyl- α -aminonitriles were subjected to Lewis acid catalysis, an unprecedented mechanistic pathway was uncovered, leading to the formation of 2,4,5-trisubstituted imidazoles via an internal cyclization sequence (Figure 1).

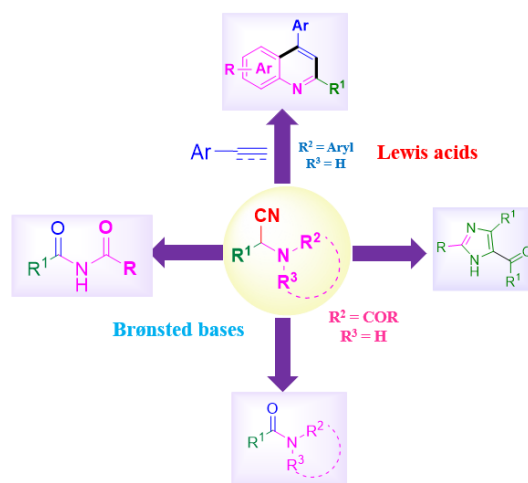


Figure 1. Overview of α -Aminonitriles under Lewis acid and Brønsted base

References:

- [1] S. Swetha & G. C. Senadi, *Adv. Synth. Catal.* 364, 2872-2882 (2022).
- [2] S. Swetha, K. Muthu, K. Govindan, N. Chen, W. Lin & G. C. Senadi, *Org. Lett.* 25, 4086-4091 (2023).
- [3] S. Swetha & G. C. Senadi, *Asian J. Org. Chem.* 12, e202300433 (2023)

Bio-Sketch of the Speaker

Dr. Gopal Chandru Senadi

Research Associate Professor

Department of Chemistry

SRM Institute of Science and Technology, Tamil Nadu, India

Phone No.: 9176226300

E-mail: chandrug@srmist.edu.in



Research Career

Dr. Gopal Chandru Senadi, known as Chandru, was born and raised in Chennai, Tamil Nadu, India. He earned his B.Sc. in Chemistry from the University of Madras (**2005**) and his M.Sc. in Applied Chemistry from Anna University (**2007**). Dr. Senadi gained over 4 years of experience in Synthetic R&D, holding positions from Senior Chemist to Senior Research Associate at GVK Biosciences and Anthem Biosciences. He completed his Ph.D. at Kaohsiung Medical University, Taiwan (**2015**), specializing in transition-metal and metal-free synthetic strategies. Following a 3-year postdoctoral fellowship funded by the National Science and Technology Council (NSTC), Taiwan, Dr. Senadi joined SRM Institute of Science and Technology in September **2018** as an Assistant Professor in the Department of Chemistry. Since February **2025**, he has been serving as a Research Associate Professor at SRMIST.

Research Interest

Our Research Team Focuses on Sustainable Molecular Transformations via

- Visible-Light Photocatalysis
- Organic Electrochemistry
- Biomass-Derived Renewable Carbon Synthons
- Heterogeneous Catalysis
- Lewis (Brønsted)-Acid Mediated Reactions and Iodide-Mediated Reactions.
- Harnessing the activity of α -aminonitriles

Awards and Recognition

- Best Employer of the Month Award at GVK Biosciences, Hyderabad, India (**2008**)
- Ministry of Science and Technology (MoST, Taiwan) Postdoctoral Award (August **2015**-July **2018**).
- Ministry of Science and Technology (MoST, Taiwan), Travel Grant Award to deliver a oral talk in 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017 (**2017**).
- Recipient of the UGC-FRPS Startup Grant (**2019**)
- Recipient of the SERB-CRG (**2022**)
- Nominated as a Member of the Board of Studies for the Chemistry courses offered to various UG programmes in the Affiliated (Non-Autonomous) Institutions under Anna University for a period of three years from **August 2025**
- Appointed as Visiting Adjunct Associate Professor at the Department of Medicinal & Applied Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan from **August 2025 to July 2028**.

Publications in Journals & Patents - 77

Details of projects handled - 03

Technology development/ Initiation

Indazole 2-oxides compound and method for preparing indazole 2-oxides compound for providing a nitrogen heterocyclic compound used as a precursor for drugs. Patent/Publication Number: I640512/Publication 201917118 (Taiwan Patent).

Others

Ph.D. Completed – 05

Ph.D. Ongoing – 06 , h-Index – 24, i10-Index – 42

<https://www.srmist.edu.in/faculty/dr-gopal-chandru-senadi/>

SL18

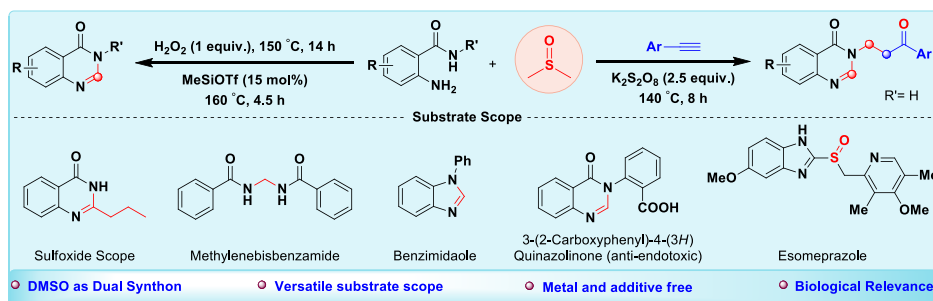
DMSO Beyond a Solvent: Sustainable Pathways to Heterocycles and Sulfoxides

¹Dr.Kishor Padala

¹Department of Chemistry, Central Tribal University of Andhra Pradesh, Vizianagaram, Andhra Pradesh, India, 535003.

Abstract:

Developing sustainable and efficient synthetic methodologies is a central goal of modern chemistry. Our work explores the unique ability of *dimethyl sulfoxide* (DMSO) to serve simultaneously as solvent and synthon, enabling green and practical access to pharmaceutically important heterocycles and organosulfur scaffolds.¹ We have established several complementary strategies. A H₂O₂-mediated annulation of 2-aminobenzamides with DMSO delivers quinazolin-4(3H)-ones under metal-free conditions.² Building on this, a TMSOTf-promoted multicomponent protocol provides rapid entry to a wide array of quinazolinones in high yields.³ In another approach, a K₂S₂O₈-driven tandem annulation of 2-aminobenzamides with terminal alkynes affords *N*-substituted quinazolinones, showcasing DMSO's role as a multiple carbon synthon.⁴ Beyond heterocycles, we have also designed a microwave-assisted oxidative condensation of aldehydes and benzyl alcohols with DMSO, producing vinyl sulfoxides efficiently under mild, additive-free conditions.⁵ Together, these methodologies highlight DMSO's versatility in promoting key C–C, C–N, and C–S bond formations without toxic metals or harsh conditions. They demonstrate how a simple, inexpensive reagent can be re-imagined as a powerful tool for eco-friendly synthesis, opening practical new pathways to heterocyclic and organosulfur chemistry of pharmaceutical relevance.⁶



Reference:

1. A Sumit. K, Ashutosh. D, Barnali. M, Soumyadip. D, Sai. D, Kishor. P, *Topics in Current Chemistry*. **2024**, 382, 36.
2. A Sumit. K, Padala. K, Maiti. B, *ACS omega*. **2023**, 36, 33058-33068 .
3. Sumit. K, Ragupathy. S, Kishor. P, and Barnali. M, *Chemistryselect.*, **2023**, 13, e202303665.
4. Ajay. U, Sumit. K, Santhosh. M, Prithvirajan. B, Anilkumar. K, Kishor. P, Annamalai. P. *Org. Biomol. Chem.*, **2025**, 23, 6801-6807.
5. Desai. B, Arti. R, Monak. P, Akshay. B, Sudha. S, Kishor. P, Togati. N. *Asian J. Org. Chem*. **2025**, 0, e00210.
6. Sumit. K, Kishor. P, *Chem. Commun.* **2020**, 56, 15101-15117.

Bio-Sketch of the Speaker

Dr. Kishor Padala,

Assistant Professor, Department of Chemistry,
Central Tribal University of Andhra Pradesh,
Vizianagaram, AP, 535003.

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Research Career

December 2022 - Till date: Assistant professor, Department of Chemistry, Central Tribal University of Andhra Pradesh (CTUAP), Vizianagaram, Andhra Pradesh, India.

Nov 2018- December 2022: Assistant Professor, Department of Chemistry, SAS, Vellore Institute of Technology (VIT), Vellore.

Nov 2016 – Nov 2018: Postdoctoral fellow at The Hebrew University of Jerusalem, Safra Campus, Givat Ram, Jerusalem 91904, Israel.

PhD.: Jan 2011- April 2016: Indian Institute of Science Education and Research (IISER), Pune (India) (PhD supervisor: Prof. Masilmani Jeganmohan)

Research Interest

DMSO-based synthesis, heterocycles (quinazolinones), green/metal-free methods, and natural product scaffolds.

Awards and Recognitions

- Associate Member of The Royal Society of Chemistry (AMRSC) – 2022
- Research Award, VIT, Vellore – 2020
- Outstanding PBC Post-Doctoral Researcher Fellowship Award, The Council for Higher Education of Israel – 2017
- CSIR-JRF Scholarship, Joint CSIR-UGC National Eligibility Test (NET), India – 2010

Publications in Journals & Patents

Publications: 24

Details of projects handled

Major projects: 2 {SERB (1), CSIR (1)}

Others: Supervision of research degrees (Ph.D.): 1

OL7

Exploration of Cyclic Enamines through Pot, Atom, and Step Economic Strategies: A Sustainable Route to Bioactive Hybrid Heterocycles

Tasneem Parvin¹

¹ Department of Chemical Science and Technology, National Institute of Technology Patna, Ashok Rajpath, Patna-800005, Bihar, India

Abstract:

Heterocyclic frameworks represent the fundamental structural motifs in a wide range of bioactive natural products, pharmaceuticals, and functional materials. The quest for efficient, sustainable, and diversity-oriented synthetic methodologies for the rapid assembly of such scaffolds continues to be a central theme in modern organic chemistry. In this context, the design and application of cyclic enamines as reactive and versatile intermediates offer a powerful platform for the construction of bioactive hybrid heterocycles. This talk will highlight our recent contributions toward the development of pot, atom, and step (PAS) economic strategies that combine synthetic efficiency, environmental sustainability, and structural diversity. The developed methodologies integrate multiple bond-forming transformations in a single operation, thereby minimizing reaction steps, reducing waste generation, and maximizing atom utilization. The reactions proceed smoothly under mild conditions using readily available substrates, green solvents, and eco-friendly catalysts, affording a broad array of heterocyclic products in excellent yields. Mechanistic studies, supported by spectroscopic and computational investigations, have provided valuable insights into the reactivity and selectivity of cyclic enamine intermediates. Overall, the talk underscores the synthetic utility of cyclic enamines and demonstrates how PAS-economic multicomponent and cascade reactions can serve as sustainable routes for the efficient construction of complex bioactive heterocyclic architectures with significant medicinal relevance.

References:

- [1] X. Shen, G. Hong, L. Wang, *Org. Biomol. Chem.* 23, 2059-2078 (2025)
- [2] Darakshan, T. Parvin, *Org. Biomol. Chem.* 23, 8075-8104 (2025)
- [3] U. Chaurasia, T. Parvin, H. M.Chandra Mouli, R. Peraman, A. Sahu, *Chem. Biodivers.* 22, e00417 (2025)
- [4] U.Chaurasia, T. Parvin, *Mol. Divers.* <https://doi.org/10.1007/s11030-025-11201-x> (2025)
- [5] Darakshan, T. Parvin, *J. Org. Chem.* 88, 6847-6856 (2023)
- [6] T. Parvin, *Top. Curr. Chem.* 381, 19 (2023)
- [7] A. Mehar, T. Parvin, *Tetrahedron* 160, 134025 (2024)

Bio-Sketch of the Speaker

Dr. Tasneem Parvin

Associate Professor and HoD
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National Institute of Technology Patna
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Research Career

Ph.D, Indian Institute of Technology Guwahati (2006-2009)
School of Chemistry, University of Manchester, UK under Exchange Programme (Sept 2007-Feb 2008)
Fast-Track Young Scientist, Indian Institute of Technology Patna (2010-2011)
Asst. Professor, National Institute of Technology Patna (June 2011-July 2018)
Associate Professor, National Institute of Technology Patna (July 2018- Till now)

Research Interest

Organic Synthesis • Methodology Development • Green and Sustainable Chemistry • Multicomponent Reactions • Heterocyclic Chemistry • Design and Synthesis of Bioactive Molecules

Awards and Recognitions

Received a letter of appreciation from Royal Society of Chemistry as Highly Cited Author in 2021 for publishing research in the top 5% of highly cited works from Indian institutions.

Citation of paper in "Scientific Background of the Nobel Prize in Chemistry in 2021"

Publications in Journals & Patents

52 Papers in peer-reviewed international journals + 5 Patents

Details of projects handled

3

Technology development/ Initiation

N/A

Others

Currently serving as the Head of the Department of Chemical Science and Technology, NIT Patna

Total Citation: 1940

H-index: 26

I10 index: 35

OL8

Synthesis and Characterization of Polymer nanocomposites for biological and photocatalytic activities

Y.Prashanthi^{1,*}, P.Uday Prakash¹

¹ Department of Chemistry, Mahatma Gandhi University, Nalgonda, Telangana, India

Abstract :

This study explores the synthesis and characterization of ZnO-based polymer nanocomposites (ZnO@CTAB-SA) employing sodium alginate (SA) and cetyltrimethylammonium bromide (CTAB) as matrices. The composites were synthesized using an in-situ polymerization method, integrating different amounts of ZnO nanoparticles. The materials exhibited substantial antibacterial effectiveness against *Staphylococcus aureus* (Gram-positive) and *Escherichia coli* (Gram-negative), in addition to antifungal activity against *Aspergillus niger*. Characterization methods including FTIR, PXRD, SEM, and EDAX validated the structural integrity and efficient dispersion of ZnO nanoparticles within the polymer matrix. Furthermore, the composites demonstrated improved photocatalytic degradation of commercial dyes, such as Rhodamine B and Alizarin Red S, facilitated by adsorption and surface contacts. These results exhibit ZnO@CTAB-SA nanocomposites as a promising multifunctional material for biomedical antibacterial approaches. Conclusion: CTAB and ZnO nanoparticles enhance the composite structure and microbial cell contact, leading to increased bioactivity. These nanocomposites effectively degrade commercial dyes like Rhodamine B and Alizarin Red S through photocatalysis, indicating their potential for wastewater treatment.

References:

- [1] Ambalgi, S. M., Inamdar, H. K., Manjula, V. T., Nagaraja, S., and Shrishail, G. (2016).
- [2] Bains, D., Singh, G., and Singh, N. (2022).
- [3] Canama, G. J. C., Delco, M. C. L., Talandron, R. A., and Tan, N. P. (2023).

CONTACT/PRESENTING AUTHOR

*Dr.Y.Prashanthi

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prashanthingu1@gmail.com

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Asst. Professor
Mahatma Gandhi University
Nalgonda, Telangana, India
Phone No.: 9010203857
E-mail: prashanthingu1@gmail.com



Research Career

17 years

Research Interest

Inorganic Chemistry, Material Science & Analytical Chemistry

Awards and Recognitions

Associate Fellow in TAS

Publications in Journals & Patents

35 publications in journals & 4 patents

Details of projects handled

4

Day3 – 19-11-2025, Auditorium 1

IL26

Harnessing Synthetic Innovation for Complex Natural Products and Therapeutic Discovery

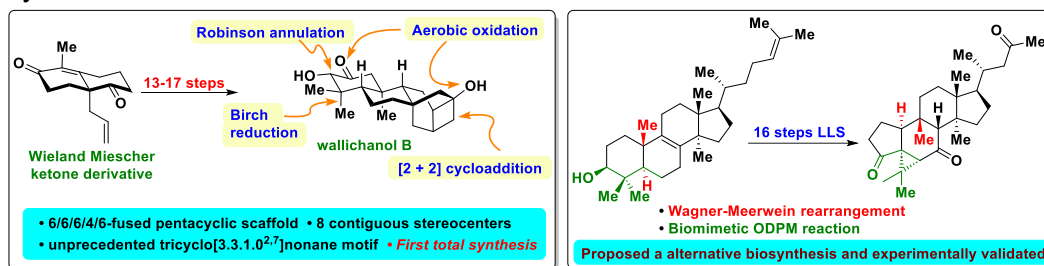
Dattatraya H. Dethe

Department of Chemistry, Indian Institute of Technology Kanpur, UP

(Email: ddethe@iitk.ac.in)

Abstract:

This presentation highlights our efforts in the enantioselective synthesis of structurally complex natural products and their therapeutic potential. We achieved the first 13-17 steps enantioselective total syntheses of rearranged *ent*-trachylobane diterpenoids, including (-)-wallichanol A, (-)-wallichanol B, and (-)-sanguinolane, via a novel intramolecular [2+2] cycloaddition, selective alkene reduction using hydrogen atom transfer, and aerobic oxidation strategies. We constructed unique pentacyclic frameworks containing a tricyclo[3.3.1.0^{2,7}]nonane motif.^{1,2} Concurrently, we explored the molecular editing of steroids to synthesize cucurbalsaminone A and its analogues, showcasing a biomimetic pathway from lanosterol. This approach incorporated oxidative olefin transposition, oxa-di- π -methane rearrangement, and selective migrations, enabling the discovery of potent antiproliferative agents targeting hepatocellular carcinoma. Mechanistic studies revealed their ability to induce oxidative cell death, offering valuable insights into the synthesis of complex triterpenoids and novel therapeutic candidates.³ Together, these projects demonstrate the power of innovative synthetic strategies in unraveling natural product complexity and advancing medicinal chemistry.



References

1. Pan, L.; Zhou, P.; Zhang, X.; Peng, S.; Ding, L.; Qiu, S. X. Skeleton-Rearranged Pentacyclic Diterpenoids Possessing a Cyclobutane Ring from *Euphorbia w Allichii*. *Org. Lett.* **2006**, 8 (13), 2775–2778.
2. Dräger, G.; Jeske, F.; Kunst, E.; Lopez, E. G.; Sanchez, H. V.; Tschritzis, F.; Kirschning, A.; Jakupovic, J. Tonantzitlone and Other Diterpenes from *Stillingia Sanguinolenta*. *European J. Org. Chem.* **2007**, 2007 (30), 5020–5026.
3. A. Mónico, C. Ramallete, V. André, G. Spengler, S. Mulhovo, M. T. Duarte, M. J. U. Ferreira, *J. Nat. Prod.* **2019**, 82, 2138–2143.
4. Dethe D. H., Singha C., Siddiqui, S. A., Biomimetic Synthesis of Cucurbalsaminone A, *Org. Lett.* **2025**, 27, 3159–3163.
5. Dethe D. H., N. Sharma and S. Juyal., Concise Enantioselective Total Synthesis of Rearranged *ent*-Trachylobane Diterpenoids (-)-Wallichanols A and B, *Angew. Chem. Int. Edn.*, **2025**, e202505766.

Bio-Sketch of the Speaker

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Dr. Jag Mohan Chair Professor

Department of Chemistry

Indian Institute of Technology Kanpur

Kanpur 208 016 (UP), INDIA

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Homepage: home.iitk.ac.in/~ddethe



Dattatraya Dethe obtained Ph.D. in synthetic organic chemistry from Indian Institute of Science, Bangalore in 2005. He subsequently held postdoctoral position in Prof. K.C. Nicolaou's group from 2005-2008. He then joined as a senior scientist in a drug discovery firm Albany Molecular Research Inc. at Singapore. He then returned back to India and joined National Chemical Laboratory, Pune as a Scientist-E1 from Aug 2009. Later in Dec 2011 he moved to IIT Kanpur and currently working there as professor in the Department of Chemistry.

His research interests include biomimetic total synthesis of natural products, asymmetric catalysis, development of metal catalysed new C-C and C-X bond forming reactions.

He is a recipient of CSIR young scientist award in Chemical Sciences (2011), OPPI young scientist award (2011), AVRA young scientist award (2014) and he was also young associate of Indian Academy of Sciences, Bangalore. He is also recipient of CRSI bronze medal 2020 and SERB-STAR Award-2020. He is also Fellow of National Academy of Sciences, FNASc. Recently he was awarded C. N. R. Rao National Prize for Chemical Sciences by CRSI.

In last 15 years he has published more than 90 research papers (1-JACS, 1-Angew. Chem., 3-Chem. Sci., 17-Org. Lett., 11-Chem. Commun., 11- JOC, 4-Chem. Eur. J., 3-Org. Chem. Front., etc) in the area of total synthesis and also has one patent to his credit.

IL27

Total Synthesis of Biologically Active Complex Alkaloids

Alakesh Bisai

Department of Chemical Sciences, IISER Kolkata, Mohanpur, WB, INDIA

e-mail: alakesh@iiserkol.ac.in**Abstract:**

The natural product chemical diversity is more closely aligned with drugs than synthetic libraries, thus making them ideal candidates for drug discovery projects.^{1a-b} Marine organisms can be considered the most recent source of bioactive natural products in relation to terrestrial plants and nonmarine microorganisms.^{2a-c} The beauty of Nature is that she produces a variety of complex natural products in entioenriched form (Figure).³⁻⁴ In the above context, naturally occurring alkaloids with impressive diversity of biological activities drew our interest for the development of bio-inspired strategies.⁵⁻⁶ Towards this, we explored Nature-Inspired strategies that will be discussed in this talk.

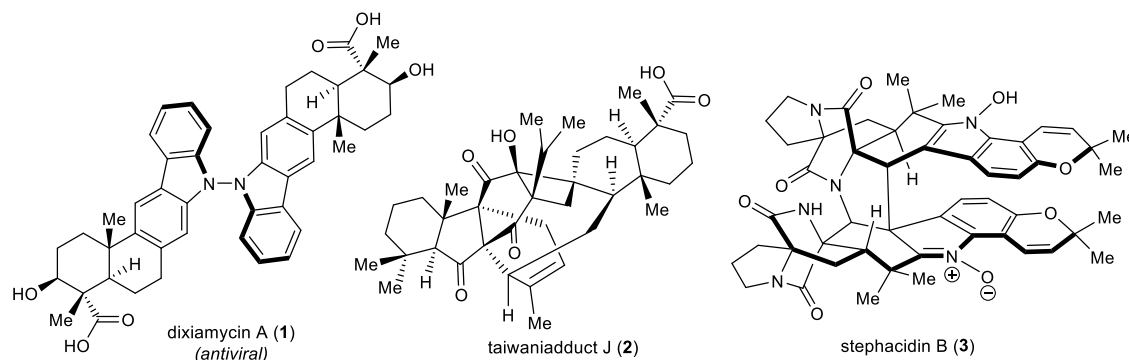


Figure. Architecturally intriguing secondary metabolites of biological relevance.

References and Notes:

- (a) C. Jiménez *ACS Med. Chem. Lett.* **2018**, 9, 959 (Marine Products in Medicinal Chemistry). (b) M. Munda, R. Nandi, S. Kundu, V. R. Gavit, S. Niyogi, A. Bisai *Chem. Sci.* **2022**, 13, 11666.
- (a) R. Nandi, S. Niyogi, S. Kundu, V. R. Gavit, M. Munda, A. Bisai *Chem. Sci.* **2023**, 14, 8047. (b) S. Niyogi, A. Mondal, M. Nandy, A. Bisai, *Org. Lett.* **2024**, 26, 8643. (c) M. Munda, A. Mondal, N. K. Roy, R. Murmu, S. Niyogi, A. Bisai *Chem. Sci.* **2024**, 15, 9164.
- (a) R. Murmu, S. Kundu, M. Majhi, S. Pal, A. Mondal, A. Bisai, *Chem. Commun.* **2024**, 60, 9737. (b) M. Nandy, A. Das, S. Niyogi, A. Khatua, D. Jana, A. Bisai, *Org. Lett.* **2024**, 26, 1531.
- (a) S. Kundu, D. Jana, N. Mandal, A. Mondal, A. Dutta, A. Bisai *Chem. Sci.* **2024**, 15, 14946. (b) S. Pal, S. Majumder, P. Shyamal, D. Mondal, B. Das, A. Bisai *Chem. Sci.* **2024**, 15, 19851. (c) D. Jana, A. Khatua, S. Noskar, M. Nandy, A. Bisai *JACS Au* **2025**, 5, 1376-1381.
- (a) N. K. Roy, R. Murmu, M. Munda, S. Niyogi, A. Bisai, *Chem. Commun.* **2025**, 61, 11053. (b) A. Mondal, A. Mondal, T. Roy, A. Bisai, *Org. Lett.* **2025**, 27, 6878.
- (a) R. Nandi, R. Murmu, S. Sadhukhan, D. Pal, S. Biswas, B. Das, A. Bisai, *Org. Lett.* **2025**, 27, 1531. (b) K. Shaw, A. Roy, D. Mondal, P. Shyamal, A. Khatua, A. Bisai, *Chem. Commun.* **2025**, 61, 12944. (c) N. K. Roy, R. Murmu, M. Majhi, S. Biswas, A. Bisai, *Org. Lett.* **2025**, 27, 9281.

Bio-Sketch of the Speaker

Alakesh Bisai, FRSC, FNASc

Professor (HAG) of Chemistry & Dean, IWD (Infrastructure)

IISER Kolkata, Nadia 741 246, WB

Former Professor & Dean, Faculty Affairs, IISER Bhopal (2009-2020)

WWW: <https://www.iiserkol.ac.in/~alakesh/alakesh.html>

PhD (2006) @ IIT Kanpur, INDIA (Supervisor: Prof. Vinod K. Singh)

Postdoc (2006 – 2009) @ UC Berkeley, CA [Advisor: Prof. Richmond Sarpong]

Independent Career:

@IISER Bhopal [(2009 – 2020) PhD Thesis Guided: 22 and MS Dissertations: 15]

@IISER Kolkata [2019 – on-going: PhD Thesis Guided: 06 and MS Dissertations: 11]

Research Focus: Strategies for Structurally Intriguing Marine Natural Product of Biological Relevance.

Research Highlights in SYNFACTS: [Narcipavlines A & B: Synfacts **2025**; 21, 115] [Codeine: Synfacts **2024**; 20, 1209]; Research Highlights in 'Organic Chemistry Portal' as 'The Bisai Synthesis of (-)-Physovernine' (**2018**); 'The Bisai Synthesis of Lycoramine' (**2023**); 'Alkaloid Synthesis: Codeine (Bisai) (**2025**); and 'The Bisai Synthesis of Oridamucin B' (**2025**).

Representative Publications:

Chem. Sci. 2022, 13, 11666; *Chem. Commun.* 2022, 58, 3929; *Chem. Sci.* 2023, 14, 8047; *ACS Catal.* 2023, 13, 2118; *Chem. Commun.* 2024, 60, 9737; *Chem. Sci.* 2024, 15, 9164; *Org. Lett.* 2024, 26, 8643; *Chem. Sci.* 2024, 15, 14946; *Org. Lett.* 2024, 26, 10803; *Chem. Sci.* 2024, 15, 19851; *Chem. Commun.* 2025, 61, 11053; *Org. Lett.* 2025, 27, 1531; *JACS Au*, 2025, 5, 1376; *Chem. Commun.* 2025, 61, 12944.

Position held:

- Professor – HAG (Higher Academic Grade) (Sept. 2025 – on-going), [IISER Kolkata](#)
- Professor (2019 - 2025): Dept. of Chemical Sciences, [IISER Kolkata](#)
- Professor (2018 - 2020): Dept. of Chemistry, [IISER Bhopal](#)
- Associate Professor (2013 – 2018): Dept. of Chemistry, [IISER Bhopal](#)
- Assistant Professor (2009 – 2013): Dept. of Chemistry, [IISER Bhopal](#)
- Post-Doctoral (2006 –2009): Dept. of Chemistry, [University of California at Berkeley](#), CA

Awards & Recognitions:

- C. N. R. Rao National Prize in Chemical Science (CRSI, 2026)
- DST Advanced Materials Research Grant (*erstwhile* DST Nano-Mission 2025)
- Fellow, The National Academy of Sciences (NASI), (FNASc, 2024)
- Fellow, [Royal Society of Chemistry](#) (FRSC), (2023)
- STARS-MoE 2023 Research Grant
- Prof. A. Srikrishna Memorial Lecture (Univ. of Hyderabad, 2022)
- 'CDRI Award' 2022 for Excellence in Drug Research (2022)
- [SERB](#), DST Special Call on 'Reagentless Chemistry' 2022
- Prof. Dhananjay Nasipuri Memorial Lecture 2021 ([Indian Chemical Society](#))
- Silver Medal, [Chintan Rasayan Sanstha \(CRS\) 2021](#) (2021)
- Fellowship, '[SERB-STAR](#)' & Research Grant (2021-2024)
- 'Bronze Medal' of the [CRSI, India](#) (2020)
- Fellow, [Indian Chemical Society](#) (FICS), (2020)
- Young Scientist Award by [CRSI](#), India (2018)
- [DST](#) Fast-Track Project (2013-2016) for Young Scientist
- Young Scientist Research Award by the BRNS, DAE (2011-2014)



SL19

Cascade Functionalization/Annulation Approaches for the Assembly of Fused-Heterocycles

Chada Raji Reddy*

Department of Organic Synthesis & Process Chemistry

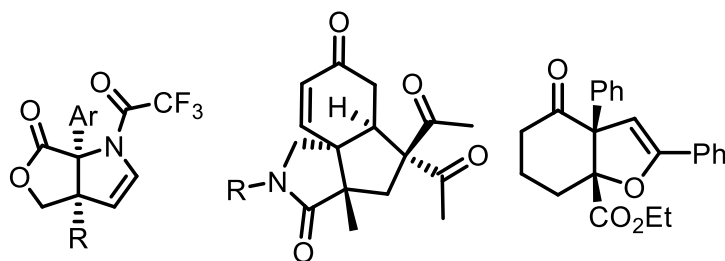
CSIR-Indian Institute of Chemical Technology

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Abstract

Heterocyclic molecules and their analogues are commonly present in bio-active natural as well as unnatural products exhibiting significant pharmaceutical activities.¹ Motivated by the importance and need to access a diverse range of heterocycles towards drug discovery program, a plethora of methods are being developed involving different approaches. Over the last one decade, the development of cascade functionalization/annulation approach has been the attention of research initiatives.² In this direction, alkynyl/alkenyl precursors are one of the convenient precursors for the construction of complex molecular scaffolds including spirocyclic or fused-heterocyclic molecules. The present lecture will focus on the recent accomplishments on cascade functionalization/annulation of alkenyl precursors for the construction of fused-heterocycles (Figure 1).³⁻⁵

Figure 1:



References:

- [1] (a) I. Pibiri, *Int. J. Mol. Sci.* 25, 9503 (2024). (b) E. Kabir, M. Uzzaman, M. *Results in Chemistry* 4, 100606 (2022).

Bio-Sketch of the Speaker

Chada Raji Reddy

Chief Scientist & Chair

Department of Organic Synthesis & Process Chemistry

CSIR-Indian Institute of Chemical Technology

Hyderabad, INDIA

E-mail: rajireddy@iict.res.in

Homepage: <https://rajireddy9.wixsite.com/my-site2>



Dr. Raji Reddy received his Ph.D. CSIR-IICT, Hyderabad (Osmania University) in 2002, followed by a post-doctoral stay at University of South Florida, Tampa, USA (2002) and subsequently to University of Mississippi, USA (2002-2005). He returned India in 2005 and joined as a principal scientist in Sai Life Sciences, Hyderabad. Later in 2006, he joined CSIR-IICT, Hyderabad as a scientist at the Department of Organic Synthesis & Process Chemistry and presently working as a Chief Scientist.

His research interests are both fundamental and applied research, include (i) the chemistry of propargylic alcohols and propiolamides; (jj) enyne-assisted annulation reactions, *ipso*-annulations and synthesis of bio-active natural products; (iii) Process development of APIs. Representative accomplishments are: processes for Favipiravir, Remdesivir, (S)-Pregabalin, key fragment of Eribulin mesylated, Bempedoic acid and TLR 7/8 agonist molecule, used as an adjuvant in COVAXIN® (COVID-19 vaccine) have been developed and transferred to pharmaceutical organizations.

He is a Fellow of National Academy of Sciences (FNASc) and Telangana Academy of Sciences (FTAS). He is a recipient of CSIR-Technology Award-2021, NASI-Reliance Industries Platinum Jubilee Award-2020, CSIR-Technology Award-2020, CRSI Bronze Medal-2018, CDRI-Drug Research Excellence Award-2017, Dr. A K Singh Memorial-Young scientist award-2014, AVRA-Young scientist award-2011 and A P Akademi-Young scientist award-2007.

He is an author of 190-publications, 15-patents, 3-review articles and 2-book chapters. Under his supervision 37-Students have been awarded Ph. D. degree. Presently, 12-research fellows are working for their Ph. D. Mentored 22-students for their Master's dissertation.

SL20

Light-Camera-Action: Shining Visible Light on Hantzsch Ester

Indranil Chatterjee*

Indian Institute of Technology Ropar, Rupnagar, Punjab – 140001, India

(Email: indranil.chatterjee@iitrpr.ac.in)**Abstract:**

When exposed to light, molecules in an electronically excited state undergo fascinating chemical reactions distinct from their behavior in the ground state.^[1] This captivating principle lies at the core of photochemistry, giving rise to unprecedented transformations. In excited state, a molecule can serve as a superior electron donor (reductant) or a more effective electron acceptor (oxidant), capabilities unattainable through conventional ground-state reactivity.^[2] The redox reaction found in almost all living cells involves the conversion between NAD⁺ and NADH. This process is essentially a hydride (H⁻) transfer reaction. In the realm of synthetic organic chemistry, the structurally similar 1,4-dihydropyridine (1,4-DHP) or Hantzsch ester has emerged as a promising hydride source in its ground state, commonly used in catalytic hydrogenation reactions.^[3] Recent research has unveiled its potential to act as a strong photoreductant or as a source of hydrogen atoms via a single electron transfer (SET) process when exposed to visible light.^[4]

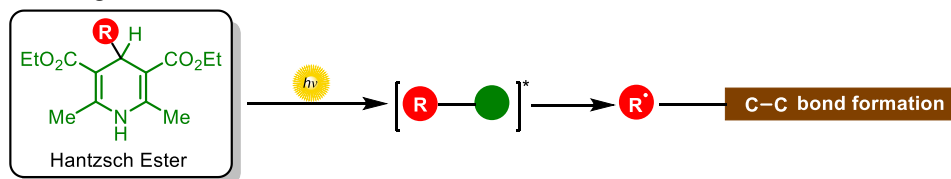


Figure 1. Graphical abstract of the generation of radicals from Hantzsch Ester

Moreover, structurally resemble, 4-alkyl-1,4-DHPs, in its excited state can act as a source of alkyl radicals without the need for any photocatalyst, and the resulting radicals can be further utilized to form C-C bonds. Inspired by the groundbreaking work of Melchiorre, Nishibayashi, and others,^[5, 6] our group has also demonstrated C(sp³)-C(sp³) cross-coupling using these 4-alkyl-1,4-DHPs.^[7] The focus of this talk will primarily center on the potential of these DHPs to reduce challenging molecules or to leverage the generated alkyl radicals to create diverse molecular complexity.

References:

1. (a) Balzani, V.; Ceroni, P.; Juris, A. *Wiley-VCH, Weinheim*, **2014**. (b) Klan, P.; Jacob, J.; *Wiley, Hoboken*, **2010**.
2. (a) Albin, A.; Fagnoni, M. *Wiley-VCH, Weinheim*, **2010**. (b) Turro, N. J.; Ramamurthy, V.; Scaiano, J. C. *University Science Books, Sausalito, CA*, **2010**.
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5. Buzzetti, L.; Prieto, A.; Roy, R. S.; Melchiorre, P. *ACS Catal.* **2018**, *8*, 1062–1066.
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Bio-Sketch of the Speaker

Prof. Indranil Chatterjee

Department of Chemistry

IIT Ropar

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Homepage:

<https://sites.google.com/iitrpr.ac.in/ic-research-group-iit-ropar/home>



Research Career

Dr. Indranil Chatterjee obtained his B.Sc. from Calcutta University, India in 2006, and then he moved to IIT Kharagpur for his M.Sc. study. In 2008 he moved to Germany for his Ph.D. study at Westfälische Wilhelms-University Muenster under the guidance of Prof. Dr. Armido Studer, where his studies centred on catalytic asymmetric cycloaddition reactions. After finishing his Ph.D. study in November 2011, he joined as a Postdoctoral fellow with Prof. Paolo Melchiorre in ICIQ, Tarragona, Spain in March 2012. His area of research mainly focused on new organocatalytic cascade reactions. From 2014 to 2016 he did another Post-Doc with Prof. Martin Oestreich at the Technische Universität Berlin, concentrating his research on Lewis acid catalysis. In December 2016 he joined IIT Ropar as an Assistant Professor. Since August 2024, he is holding a position of Associate Professor at the Indian Institute of Technology Ropar, India.

Research Interest

Photoredox catalysis, Asymmetric catalysis, Transition-metal catalysis, Visible-light mediated Organic Transformations

Awards and Recognitions

- (i) Institute Best Teaching Award (2020).
- (ii) Thieme Chemistry Journal Award, 2022.

Publications in Journals & Patents

50

Details of projects handled

04

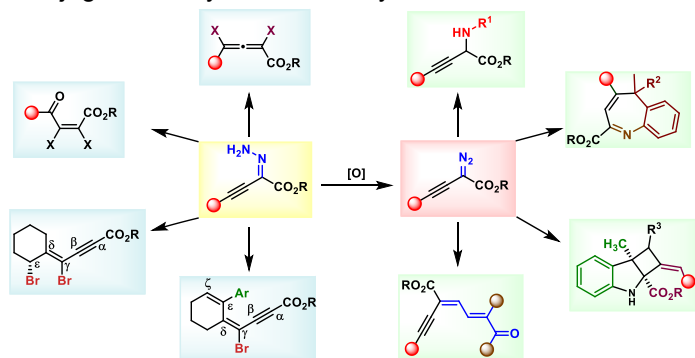
SL21

Exploring the Reactivity of Alkynyl Hydrazone and Diazo Carboxylates for the Synthesis of Diverse Scaffolds

Guru Brahamam Ramani^{1*}

¹Department of Chemistry, Indian Institute of Technology Jammu, NH-44, PO Nagrota, Jagti, Jammu and Kashmir, 181221, India

Hydrazones are among the most versatile building blocks in organic synthesis, valued for their accessibility, stability, and broad reactivity profile. Alkynyl hydrazones, which possess a conjugated alkyne–hydrazone structure, display unique electronic properties and ambiphilic reactivity that facilitate a wide range of molecular transformations. In exploration of the reactivity of alkynyl hydrazones, we developed a practical route for the synthesis dihaloallenoates and dihaloenates via an electrophilic halogenation with *N*-halosuccinimides.¹ Furthermore, we attempted the first remote electrophilic bromination of enynyl hydrazone carboxylates. Interestingly, this transformation delivers stereodivergent γ -brominated bromoenynoates and (γ,ϵ)-dibromoenynoates in good to excellent yields with high stereoselectivity, wherein the product geometry is governed by the substitution in the hydrazone backbone. On the other hand, the alkynyl hydrazones were oxidized to diazo acetates, which were utilized in carbene transfer reactions. We have recently established a protocol for alkyne carbene insertion into N–H bonds using Rh-catalysis, which yields α -alkynyl- α -amino esters.² Delightfully, the 2-alkenyl-*N*-propargylanilines obtained via the insertion of 2-alkenylanilines undergo cyclization to yield benzo[*b*]azepines frameworks when subjected to thermal conditions. Whereas the same propargylamine intermediates can isomerize under basic conditions to form allenoates, which then undergo cycloaddition to yield indoline-fused cyclobutane scaffolds. The dual reactivity of alkyne and diazo functional groups underscores the synthetic versatility of alkynyl diazoacetates, broadening their potential in the construction of diverse molecular architectures under mild reaction conditions. Additionally, we also developed the first visible-light-driven alkynyl carbene insertion into furans, providing a stereoselective synthesis of π -enriched conjugated dienynals and dienynones with excellent selectivity.³



References:

- [1] a) Sharma, A.; Jamwal, P.; Gurubrahamam, R. *Org. Lett.* 25, 7236–7241 (2023). b) Jamwal, P.; Sharma, A.; Gurubrahamam, R. *Org. Lett.* 25, 6607–6612 (2023).
- [2] Sharma, A.; Vaid, H.; Kotwal, R.; Mughal, Z. N.; Gurubrahamam, R. *Org. Lett.* 26, 4887–4892 (2024).
- [3] Jamwal, P.; Shukla, R.; Gurubrahamam, R. *Org. Lett.* 27, 11163–11168 (2025).

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Research Career

MSc (2006) and Ph.D. (2013): School of Chemistry, University of Hyderabad.

Postdoc-1 (2013-2017): National Taiwan Normal University, Taipei, Taiwan.

Postdoc-2 (2017-2019): Stockholm University, Stockholm, Sweden.

Industrial experience (2019): Syngene International Ltd., Bangalore.

Assistant Professor (2019/10 onwards): Department of Chemistry, IIT Jammu.

Research Interest

Catalysis, Hydrazone and Diazo Chemistry, and Photochemistry.

Publications in Journals & Patents

33

Details of projects handled

04

SL 22

Two Tales of C–H Functionalization

Sandip Murarka*

Department of Chemistry, Indian Institute of Technology Jodhpur, Rajasthan.

E-mail: sandipmurarka@iitj.ac.in

Abstract:

The robust, predictable, chemo- and site-selective conversion of a C-H into a C-X (X = carbon and heteroatom) bond represents the holy grail in organic chemistry.¹ Moreover, direct C-H functionalizations play a pivotal role in developing new chemical entities (NCEs) and drug discovery processes as they enable rapid diversification of pharmaceutical molecules to an exciting range of closely related bioactive analogs and thus allow access to unexplored regions of chemical space. Along these lines, we have recently achieved an unprecedented and synthetically challenging selective *meta*-C–S bond formation on anilines using CS₂ and amines via an *in situ* generated dithiocarbamate as the sulfur source.² Moreover, visible light-induced synthesis provides a sustainable platform to achieve direct C-H functionalizations under mild conditions. Accordingly, our group has developed a photoinduced site-selective method for the direct Csp³-H arylation and alkylation of glycine derivatives, and peptides in a site-selective manner using diaryliodonium reagents (DAIRs) as aryl radical progenitors and halogen-atom-transfer (XAT) mediators under visible light irradiation.³ Notably, we have also achieved the direct site-selective Csp³-H alkylation of glycines and peptides employing feedstock carboxylic acids as alkyl radical precursors via an novel iron-photocatalyzed ligand-to-metal charge transfer (LMCT) pathway.⁴

References

- [1] (a) T. Cernak, K. D. Dykstra, S. Tyagarajan, P. Vachal & S. W. Krska, *Chem. Soc. Rev.* 45, 546 (2016); (b) R. Budhwan, S. Yadav & S. Murarka, *Org. Biomol. Chem.* 17, 6326 (2019).
- [2] S. K. Parida, S. Sanghi, A. Mondal, N. Choudhary, P. Meher, P. Singh & S. Murarka, *ACS Cent. Sci.* (2025). (DOI: 10.1021/acscentsci.5c01231)
- [3] P. Meher, M. S. Prasad, K. R. Thombare, & S. Murarka, *ACS Catal.* 14, 18896 (2024).
- [4] S. P. Panda, M. S. Prasad, P. Meher & S. Murarka, *Chem. Sci.* (2025). (DOI: 10.1039/D5SC07730C)

Bio-Sketch of the Speaker

Prof. Sandip Murarka

(Department of Chemistry, Indian Institute of Technology Jodhpur, Rajasthan)

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Research Career

Dr. Murarka pursued his PhD from WWU Münster under the supervision of Prof. Armido Studer. After completing his Ph.D. (2013), he worked as a Max-Planck postdoctoral research fellow in the laboratory of Prof. Herbert Waldmann at Max Planck Institute of Molecular Physiology, Dortmund (2013-2016). Following a year long stay (2016-2017) as a Team Leader in a reputed pharmaceutical company, Syngene International Limited, he decided to return to academia. In May 2017, he joined the Indian Institute of Technology Jodhpur, India, as an Assistant Professor and was promoted to the post of Associate Professor in June 2022.

Research Interest

Dr. Murarka's current research activities include the study of novel activation modes and the development of chemoselective and sustainable synthetic transformations. His research group utilizes sustainable chemical tools, such as base-metal catalysis, photocatalysis, and electro-organic synthesis, to convert feedstock chemicals to value-added compounds and pharmaceutically relevant molecular architectures.

Awards and Recognitions

He is a recipient of the Humboldt Fellowship for Experienced Researchers (2025) by AvH Foundation, CRSI Bronze Medal (2026) by CRSI, Institute Award for Research Excellence (2025) by IIT Jodhpur, Institute Senior Researcher Award (Science Category) (2024) by IIT Jodhpur, The Early Career Research Award (2018) by SERB, Thieme Chemistry Journal Award (2022) by Thieme, and Merck Young Scientist Award (2023) by Merck. He is an Early Career Advisory Board Member (ECAB) of several journals, such as ChemistrySelect (Wiley-VCH), Chemistry an Asian Journal (Wiley-VCH), and Organic Chemistry Frontiers (RSC). He is also a Fellow of the Royal Society of Chemistry (FRSC), and Indian Chemical Society (FICS).

Publications in Journals & Patents

57 & 4

Details of projects handled

5

SL23

Taming Alkyl Boronic Esters in Cross-Couplings via Amino Radical Transfer (ART)

Srikrishna Bera

Indian Institute of Technology Tirupati, Tirupati, India.

Abstract:

Metal-catalyzed cross-couplings of aryl boron reagents, exemplified by the Suzuki–Miyaura¹ and Chan–Lam² reactions, are indispensable in organic synthesis. In contrast, analogous couplings with alkyl boronic pinacol esters (Bpins) are hindered by β -hydride elimination, isomerization, and protodeborylation. In this talk, I will discuss the amino radical transfer (ART) strategy, which converts alkyl Bpins into alkyl radicals, enabling metal-catalyzed couplings with amines, sulfenamides, and heteroarenes to access medicinally relevant scaffolds.

References:

- [1] N. Miyaura & A. Suzuki, Chem. Rev. 95, 2457–2483 (1995).
- [2] M. J. West, J. W. B. Fyfe, J. C. Vantourout, A. J. B. Watson, Chem. Rev. 119, 12491–12523 (2019).
- [3] S. Shil, B. P. Patra, T. Begam, S. Bera, J. Am. Chem. Soc. 147, 26486–2649 (2025)

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Bio-Sketch of the Speaker

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Research Career

Assistant professor: 01.2022 to now

Postdoc: 01.2018 to 12.20221; Advisor: Prof. Xile Hu at EPFL

PhD: 10.2013 to 12.2017; Advisor: Prof. Armido Studer at University of Muenster

Research Interest

Asymmetric Catalysis, Radical Chemistry, and Molecular Editing

Awards and Recognitions

Selected as one of the Early Career Researchers (ECR) by the NOST council, India.

Publications in Journals & Patents

S. Shil, B. P. Patra, T. Begam, S. Bera, J. Am. Chem. Soc. 2025, 147, 26486–26495

S. Bera, C. Fan, X. Hu, Nat. Catal. 2022, 05, 1180–1187

S. Bera, R. Mao, X. Hu, Nat. Chem. 2021, 13, 270–277

SRG-SERB (2022-2024)

SL 24

Palladium-Catalyzed Site-Selective C–H Functionalization of Arenes(Hetero), Alkenes via a Cross-Coupling Approach

Dongari Yadagiri^{1*}

¹Laboratory of Organic Synthesis and Catalysis, Department of Chemistry
Indian Institute of Technology, Roorkee, Uttarakhand-247667, India.

*E-mail: yadagiri.dongari@cy.iitr.ac.in

Introduction of functional groups onto the organic molecules is a fundamental reaction, and they are considered instrumental structural motifs in chemistry.¹ To introduce a functional group through the C–H functionalization is one of the fascinating topics in organic chemistry because, in a single step, one can introduce functional group complexity. However, a suitable directing group or specially designed substrate is needed in most cases to achieve the site-selective C–H functionalization. Otherwise, it would lead to more than one product. To overcome this problem, the thianthrenium salts are used to increase positional selectivity, readily available from the arenes and thianthrene S-oxide.² Using this concept, explored the introduction of various functionalities with the help of photo-redox chemistry and transition-metal mediated chemistry; however, Site-selective C–H functionalization with carbenes has not been developed so far via a cross-coupling approach. Here, we introduce nitrile and carbamoyl on the arenes and alkenes in a single step through a site-selective manner³ via the Pd-catalyzed cross-coupling approach of isonitriles with thianthrenium salts, which are derived from arenes, heteroarenes, and alkenes. The scope and limitations of the site-selective cross-coupling approach will be discussed during the presentation.



References:

1. Larock, R. C. *Comprehensive Organic Transformations: A Guide to Functional Group Preparations*; VCH Publishers: New York, 1989.
2. Berger, F.; Plutschack, M. B.; Riegger, J.; Yu, W.; Speicher, S.; Ho, M.; Frank, N.; Ritter, T. *Nature* **2019**, *567*, 223–228.
3. Happy, S.; Saleem, M.; Yadagiri, D. *ACS Catalysis*, **2025**, *15*, 13401-13411.

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Assistant Professor

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Biography

Native place; Nalgonda district, Telangana, India

BSc: Osmania University, Telngana, India

MSc: Kakatiya University, Telngana, India

Research Career

- Ph.D: Indian Institute of Technology Madras, Chennai, India with Prof. Pazhamalai Anbarasan
- Postdoc: The University of Illinois at Chicago and The University of Texas at Dallas, USA with Prof. Vladimir Gevorgyan
- Assistant Professor: May-2021 onwards Department of Chemistry IIT Roorkee, Roorkee, India

Research Interest

- Organic Synthesis and Catalysis
- Carbene and Metallocarbene Chemistry
- Site-selective C–H functionalization
- Light induced organic transformations

Awards:

- DST-INSPIRE faculty fellowship award from DST, Government of India
- Received Eli Lilly and Company Asia Outstanding Thesis Award 2016
- Received Prof. C. N. Pillai Prize for Best Ph.D Thesis of the Year in the Department of Chemistry (2015-2016), Indian Institute of Technology Madras
- Institute Pre-Doctoral Fellowship, Indian Institute of Technology Madras, Chennai, India - 2015
- Received Best Oral Presentation Award in CiHS-2013, Indian Institute of Technology Madras

OL10

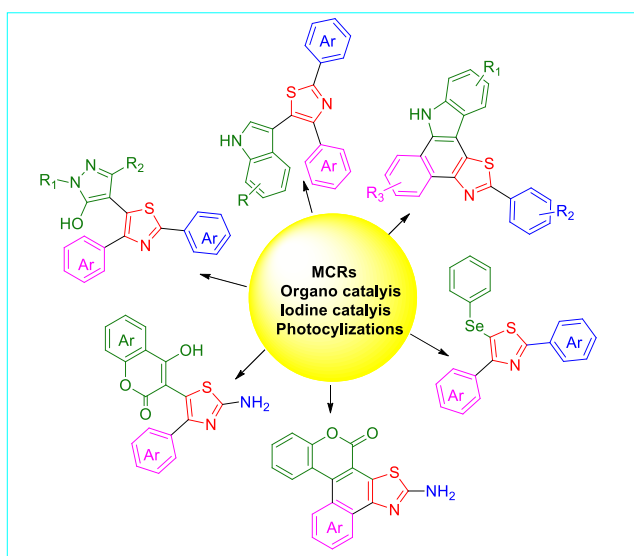
Rational Design and Green Synthetic Paradigms for the Synthesis of Substituted and Fused Thiazole Derivatives

Lokman H. Choudhury^{1,*}

¹ Department of Chemistry, Indian Institute of Technology Patna, Bihta, Patna-801106, INDIA

Abstract:

Substituted thiazoles and their fused analogues constitute indispensable structural units in medicinal chemistry, natural products, and advanced functional materials. Their unique electronic and hydrogen-bonding properties, coupled with broad pharmacological relevance, have spurred continued interest in developing efficient, selective, and sustainable routes to their synthesis. This lecture will explore the development of some new synthetic methodologies by our group employing metal-free one-pot strategies for the efficient construction of diverse trisubstituted thiazoles and fused thiazole derivatives. Emphasis will be placed on reaction design, substrate selection, and catalytic approaches that streamline synthesis and enhance molecular complexity.



References:

- [1] P. Bhaumick, R., Kumar, S. Acharya, T. Parvin, L. H. Choudhury, *J. Org. Chem.* 87,11399–11413 (2022)
- [2] R. Banerjee, D. Ali, N. Mondal, L. H. Choudhury, *J. Org. Chem.* 89,4423–4437 (2024).
- [3] P. Bhaumick, N. Mondal, L. H. Choudhury, *Eur. J. Org. Chem.* 27, e202400972 (2024)
- [4] D. Ali, N. Mondal, L. H. Choudhury, *J. Org. Chem.* 90, 8903–8916 (2025)
- [5] N. Mondal, S. Raj, L. H. Choudhury, *J. Org. Chem.* 90,14565–14578 (2025).

Bio-Sketch of the Speaker

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Indian Institute of Technology Patna
Bihta, Patna 801106
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E-mail: lokman@iitp.ac.in



Research Career

Ph.D, Indian Institute of Technology (2007)
Royal Society Postdoctoral Fellow, The University of Manchester, UK (Sep 2007- Feb 2008)
Asst Professor, North Eastern Hill University (Jan 2007-Feb 2009)
Asst. Professor, Indian Institute of Technology Patna (Feb 2009-Dec 2015)
Associate Professor, Indian Institute of Technology Patna (Dec 2015-Feb 2022)
Professor, Indian Institute of Technology Patna (Feb 2022- till now).

Research Interest

Green Chemistry, Multicomponent Reactions, Light Mediated Reactions, Catalysis, Methodology Development

Awards and Recognitions

Editorial Board Member: Scientific Reports
Recipient of Certificate of Appreciation from the Royal Society of Chemistry for publishing research in the top 5% of highly cited works from Indian institutions (year 2021).
Recipient of CAS REGISTRY, INNOVATOR certificates from the Chemical Abstracts Service, American Chemical Society

Publications in Journals & Patents

80 Papers in peer-reviewed international journals

Details of projects handled

3

Others

Served as Head, Department of Chemistry, IIT Patna
Head, SAIF IIT Patna
Member, Board of Governors and Finance Committee, IIT Patna

OL11

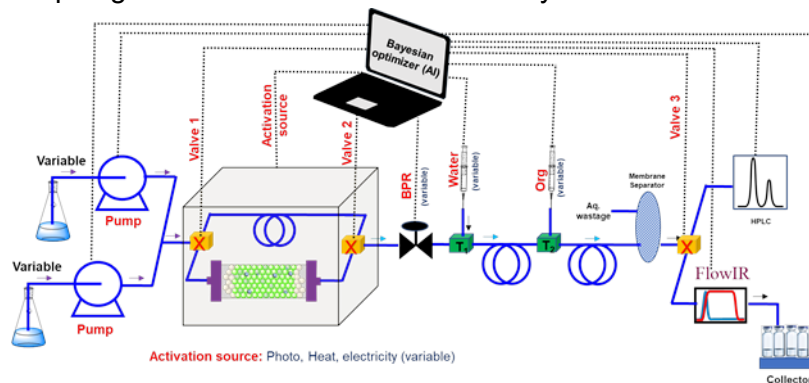
Transitioning from Batch chemistry to Flow and Digitally Programmed Chemical Synthesis

Ajay K Singh

CSIR-Indian Institute of Chemical Technology, Hyderabad

Abstract:

It is well documented that the equilibrium state of the isomeric structures is controlled by certain numerical variables such as thermodynamics, kinetics, mixing, solvent polarity, etc., and discrete variables such as catalysts, bases, acids, moisture-free conditions, and more. Optimizing these parameters is crucial. However, most graduate researchers tend to run intuition-driven experiments, such as reaction discovery and substrate scopes, rather than fully optimizing their processes to achieve industrially favorable methodologies. The current setup can be used to obtain optimal reaction conditions for desired outcomes (reaction yield, selectivity, E-factor, etc.). It is user-friendly and represents a possible solution to unify several fields (chemistry, process engineering, computer science). This setup can be used for conducting automated design of experiments (DoE) or kinetic studies, screening every combination of reaction variables in high-throughput experimentation (HTE), or utilizing self-optimization. As AI-connected laboratories become more diversified in skillsets and more interdisciplinary research is conducted, familiarity with these techniques must be embraced. Undergraduate and postgraduate courses will undoubtedly reflect this trend in the coming years.



References:

- [1] Singh et al, Org. Process Res. Dev., **2025**, 29 (3), 881-888.
- [2] Singh et al, Chem. Commu., 2024, 60 (96), 14212-14215.
- [3] Singh et al, Commun. Chem., 2024, 7 (1), 251.
- [4] Singh et al, Advance Science, **2025**, e07915.
- [5] Singh et al, Chem Asian J, **2025**, e202400438.
- [6] Singh et al, React. Chem. Eng., 2024,9, 2427-2435.
- [7] Singh et al, IN Patent App. N0170NF2025.
- [4] Singh et al, IN Patent App. 0306NF2,024

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Research Career

I obtained my Ph.D. in 2012 from the University of Gorakhpur, India. Following my doctoral work, I joined CSMCRI, Bhavnagar, where I completed my SRF and SRF-Extended tenures. I subsequently pursued postdoctoral research under Prof. Dong-Pyo Kim at Pohang University of Science and Technology (POSTECH), South Korea. Thereafter, I joined CSIR–Indian Institute of Chemical Technology (IICT), Hyderabad, as a DST-Inspire Faculty/Scientist, and later advanced to Senior Scientist. I am currently serving as a Principal Scientist at CSIR-IICT.

Research Interest

Work in our laboratory is focused on developing Continuous flow process and automation technology that are highly efficient and of broad utility. The autonomous integrated platform to develop new kinds of organic building blocks and material for energy, water, drugs, catalysis, and sensor application.

Awards and Recognitions

- DST-SRA fellowship-2022.
- Excellent grade in DST-ECR project.
- Award of Honour, Distinguished speaker at Flow Chemistry India 2018.
- Assistant Prof. of the Academy of Scientific and Innovative Research (AcSIR), 2017.
- Award of Honour, Distinguished speaker at Flow Chemistry India 2017.
- Early Career Research Award-2017.
- DST-Inspire Faculty-Jan 2016.
- “Best Paper Award 2015” of BK21 PLUS, Korea.
- ITMO University Post-Doctoral Fellowship-2015, Petersburg, Russia.
- Excellent Paper Presentation Award (Korean Society of Industrial and Engineering Chemistry-2014).
- CSIR SRF(ext) 2012, India.

Publications in Journals & Patents

59

Details of projects handled

22

OL13

Wiley's Journals and Today's Publication Landscape

Dr. Subhabrata Mukhopadhyay
Deputy Editor, Wiley

Abstract:

This talk will feature Wiley as a publishing house and its variety of journals. I'll talk about the thematic special collection '**From Molecules to Materials: Progress in Technology driven by Chemistry**' and the journals participating in the special collection. Artificial intelligence-based generative language learning programs are creating a prominent impact on the publication landscape. The scope of ethical use of AI tools in scientific peer-reviewed publications will be discussed in the talk.

Biography

Subhabrata is working with the Wiley global team from India as a deputy editor. His primary focus is on the journals, **Chemistry - An Asian Journal**, **ChemNanoMat**, and **ChemPlusChem**. Additionally, he assists in developing new editorial policies and projects. Subhabrata has a strong background in materials chemistry, with a PhD from the University of Hyderabad (2020). Before joining Wiley, Subhabrata was working at the Research Institute of Sweden (RISE), as a scientist. He also has postdoctoral experience at Ben Gurion University in Israel (2020-2022) and Uppsala University in Sweden (2022-2023).



