

IL-1

10-13 December 2023

Catalysis : a Key For Green Access to Polypyridines, Fused Heterocycles, And Phosphines via C-H Bond Functionalization

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Pyridines are key ligands to promote selective catalytic reactions, including photocatalysis, whereas phosphine ligands can create the activity of molecular metal catalysts for numerous useful catalytic reactions with green processes. Fast modifications of these pyridine and phosphine ligands via C-H bond activation/functionalization^[1] have potential to quickly create more efficient catalysts for useful applications. Several aspects of functionalization of pyridines, N-heterocycles and phosphines from catalytic C-H bond functionalizations and of recent improvements of Phosphine-Metal catalysts will be presented.

(i) Pyridines and Heterocycles

-Ruthenium(II) catalysts in water solvent without surfactant can promote sp²C-H bond activation to produce polyheterocycles, hexapyridine compounds and hexa(heteroaryl)benzenes leading to simple Ru(II) or Pd(II) complexes and catalysts.^[2]

-Ruthenium(II) catalysts can be driven for partial reduction of N-Heteroarenes for tandem functionalization via diastereoselective Annulation of Azaarenes into Fused N-heterocycles.^[3] Whereas heterogeneous Cobalt systems open the road to new heterocycles and NHC Precursors.^[4]

(ii) Phosphines

-Ruthenium(II)-catalyzed selective sp²C-H bond alkylations with alkenes of arylphosphine oxides can be controlled to give access to bifunctional phosphines with carboxylic group.^[5]

-Rhodium(I) catalysts promote the regioselective mono or dialkylation and dialkenylation of the biaryl ortho'C-H bonds of phosphines to produce functional dialkylated phosphines even with long chain;^[6] or bulky dialkenylphosphines.^[7]

Examples of increased activity of catalysts using modified phosphines will be presented for green processes: carboxylation with CO₂ of arylhalides or for C-N bond cross couplings.^[6,7]

References

[1] P. B. Arockiam, C. Bruneau, P. H. Dixneuf, *Chem. Rev.* 2012, *112*, 5879.

[2] F. Pozgan and M. Drev et al Org. Lett. 2018, 20, 5268.

[3] H. Zhao, Y. Wu, Z. Tan, H. Jiang, P. H. Dixneuf, M. Zhang, *Nature Commun.* **2022**, *13*, 2393

[4] J. -L. Sun, C. Ci, H. Jiang, P. H. Dixneuf, and M. Zhang, *Angew. Chem. Int. Ed.* **2023**, e202303007.

[5] C. S. Wang, P. H. Dixneuf, J. F. Soulé, *ChemCatChem*, **2017**, *9*, 3117.

[6] Z. Zhang, P. H. Dixneuf, J. F. Soulé, Angew. Chem. Int. Ed., 2019, 58, 14110.

[7] Zhuan Zhang, Marie Cordier, P. H. Dixneuf, J. F. Soulé. Org. Lett. 2020, 22, 5936.



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Pierre H. Dixneuf, Professor of organometallic chemistry at the University of Rennes started to create a Catalysis group in 1985. He successively developed selective catalytic transformations of alkynes, incorporation of CO₂, ruthenium-vinylidenes and -allenylidenes in catalysis, enantioselective hydrogenation for industry with chiral Ru catalysts, new alkene metathesis catalysts for the transformation of plant oil derivatives. He is now contributing since 2007 to catalytic C–H bond activation/functionalization, even in water, via sustainable processes, using mostly Ru(II) and Rh(I) catalysts and recently for the modification of polypyridines, heterocycles and phosphine ligands for the improvement of catalysts.

He has co-authored 480 publications and reviews, 120 dealing with Green C-H bond modifications, and co-edited 7 books. He received international prizes from Germany,

Italy, Spain, Portugal, China, Taiwan, India, and from French académie des sciences. He has developed cooperation with India : Coorganized 2 bilateral Cefipra symposia, in 2014 and 2015, given 2 master courses in 2016 & 2019, received 3 awards from India : B. D. Tilak lectureship from NCL Pune 2014, first Asima Chatterjee International award, Calcutta 2020, and National Academy Sciences India membership 2020. He has 17 publications with Indian students and researchers. After his work as Scientific Deputy Director of CNRS Chemistry in Paris (1996-1999), he founded the CNRS-UR1 research Institut de chimie de Rennes in 2000 and was university of Rennes vice-president for research (2001-2004).



IL-2

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Formic acid and CO as key 'power molecules' in the catalytic conversion of CO_2 to chemicals

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The chemical industry is heavily dependent on oil-based resources, the latter being required for the synthesis of 87% of chemicals in 2016.^{1,2} Accessing other chemicals directly from CO₂ would require synchronizing reduction and functionalization, which is difficult to control. An interesting intermediate would be carbon monoxide (CO) that can provide access to functionalized chemicals at a more reduced oxidation state, +II. In this lecture, I will discuss our recent

progresses in CO chemistry aiming at developing novel carbonylation reactions with ideal atom economy and coupling CO production from CO₂



with its downstream use in catalysis.³⁻⁵ Key transformations highlighting the potential of formic acid as a sustainable source of carbon and hydrogen will be presented.⁶⁻⁸

References

[1] dena (German Energy Agency), Feedstocks for the chemical industry, 2019.

[2] (a) Food and Agriculture Organization, *Journal*, 2019; (b) A. Bazzanella and D. Krämer, *Technologies for sustainability and climate protection – chemical processes and use of CO*₂, DECHEMA, 2019.

[3] T. Nasr Allah, S. Savourey, J.-C. Berthet, E. Nicolas and T. Cantat, *Angew. Chem. Int. Ed.*, 2019, **58**, 10884-10887.

[4] T. Nasr Allah, L. Ponsard, E. Nicolas and T. Cantat, *Green Chem*, 2021, DOI: 10.1039/D0GC02343D.

[5] L. Ponsard, E. Nicolas, N. H. Tran, S. Lamaison, D. Wakerley, T. Cantat, M. Fontecave, *Chemsuschem* 2021, **14**, 2198-2204.

[6] A. Imberdis, G. Lefèvre, T. Cantat, Angew. Chem. Int. Ed., 2019, 58, 17215-17219.

[7] Savourey, S.; Lefevre, G.; Berthet, J. C.; Thuery, P.; Genre, C.; Cantat, T., *Angew. Chem., Int. Ed.* 2014, **53** (39), 10466-10470

[8] Crochet, E.; Anthore-Dalion, L.; Cantat, T., Angew Chem Int Edit 2023, e202214069.



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Thibault Cantat is a group leader at the Alternative Energies and Atomic Energy Commission (CEA) in France. He obtained his Ph.D. in Chemistry in 2007 at the Ecole Polytechnique, France. Afterwards, he received a joint Director's Postdoctoral position at Los Alamos National Laboratory in the groups of Drs. Jaqueline Kiplinger, Enrique Batista and P. Jeffrey Hay. Upon returning to France in 2009, he started a research group focused on the activation and recycling of CO₂, depolymerization of wood lignin and mechanistic investigations using experimental and computational chemistry, at CEA Saclay. He has published 104 research articles (h-index=42). For his contribution on CO2 chemistry, he was awarded the Grand Prix Scientifique of the Louis D. Foundation by the Institut de France (2013), which is the most endowed research prize in France. He obtained a Starting Grant in 2013 and a Consolidator Grant in 2018 from the European Research Council and in 2014, he was a granted a Green Chemistry for Life research grant from UNESCO and IUPAC. In parallel, he provides scientific advice to policy makers and was nominated panel member at the CCUS workshop for Mission Innovation. In 2017, he was an expert and co-author of a report on Carbon Capture and Utilization for the Scientific Advice Mechanism, SAPEA, commissioned by the European Commission. Since 2020, he is the Program Leader on the Carbon Circular Economy at CEA (incl. biofuels, Power-to-X and biomass conversion technologies).



IL-3

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Catalytic' NADP⁺/NADPH Cofactor Analogues Joyanta Choudhury

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In the Calvin cycle, the atmospheric CO₂ is "fixed" (reduced) into sugars. Here, the reduced nicotinamide adenine dinucleotide phosphate (NADPH) acts as the hydride transfer (HT) cofactor to reduce the "captured" CO₂ molecule (in the form of 1,3-bisphosphoglycerate) into glyceraldehyde-3-phosphate, which is further utilized for biosynthesis of sugars and biomass. In the presence of sunlight, ferredoxin-NADP⁺ reductase (FNR) catalyzes the regeneration of NADPH from the oxidized NADP⁺ cofactor by the transfer of electrons and protons from photosystem I (PS I), where water acts as the terminal source of proton and electron. Thus, in a sense, the cofactor NADPH acts like a "catalyst" for CO₂ reduction with the help of a suitable electron/proton supply chain. Chemists target to develop synthetic analogues of the natural NADPH cofactor. Unfortunately, despite extensive investigation over decades, all synthetic NADPH model compounds/analogues (AH) developed so far, only act as "*stoichiometric*" reductant for the reduction of CO₂. The main bottleneck for their "catalytic" use has been their inefficient regeneration from the corresponding oxidized forms (NADP⁺ versions) through 2e⁻/1H⁺ transfer chemistry. This is due to several fundamental challenges such as (i) facile irreversible dimerization of the one-electron reduced radical species (A[•]), (ii) difficult protonation of the one-electron-reduced radical species (A[•]), and (iii) instability of the anionic species (A^{-}) generated through high-potential injection of the second electron $(A \rightarrow A^{-} \rightarrow A^{-})$ to the radical species (A). Optimum hydricity (ΔG_{H-}) and self-exchange reorganization energy (λ_{AH}) of the hydrides are the other key issues for effective HT reactions. Recently, by employing our in-house well-developed Rh-catalyzed 'rollover annulation' protocol,^[1] we synthesized a unique class of dicationic heterohelicenes empowered with redox-active imidazolium-fused central pyridine motif. Capitalizing their unique structural and electronic attributes, we exploited the NADP+/NADPH-like hydride-transfer redox cycle with these bis-imidazolium-embedded heterohelicenes for CO₂ reduction and similar reduction reactions in a "catalytic" manner.^[2-3] The chemistry involved in this discovery will be discussed in the presentation.

References

[1] (a) Ghorai, D.; Dutta, C.; Choudhury, J. ACS Catal. 2016, 6, 709–713. (b) Karak, P.; Dutta, C.; Dutta, T.; Koner, A. L.; Choudhury, J. Chem. Commun. 2019, 55, 6791–6794. (c) Karak, P.; Rana, S. S.; Choudhury, J. Chem. Commun. 2022, 58, 133–154. (d) Karak, P.; Choudhury, J. Chem. Sci. 2022, 13, 11163–11173.

[2] Karak, P.; Mandal, S. K.; Choudhury, J. J. Am. Chem. Soc. 2023, 145, 7230–7241.

[3] Karak, P.; Mandal, S. K.; Choudhury, J. J. Am. Chem. Soc. 2023, 145, 17321–17328.



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Joyanta Choudhury obtained Ph.D. in 2006 from IIT Kharagpur, India working under Professor Sujit Roy on the development of Ir-Sn heterobimetallic complexes for aromatic C–H functionalization. He then moved to The Scripps Research Institute, Florida, USA for postdoctoral work with Professor Roy A. Periana in the field of CH₄-to-CH₃OH (MTM) conversion chemistry. In 2008, he received Marie Curie International Incoming Fellowship from the European Union and went to the Weizmann Institute of Science, Israel to work with Professor Milko E. van der Boom on redox-active molecular assemblies on solid surfaces. He joined the Department of Chemistry, IISER Bhopal, India in 2011.

His research group at IISER Bhopal works primarily on (a) developing new reactions involving "*metal-NHC*" intermediates for the creation of task-specific functional molecules, (b) circular catalysis with CO₂, H₂ and biomass-derived energy carriers toward alternative fuels, and (c) reversible energy storage and delivery.

Award: Chemical Research Society of India, Bronze Medal (2019)



IL-4

10-13 December 2023

π-Acceptor Caged Phosphine Ligands: Exploration of Novel Catalytic Reactivity and Mechanism

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Phosphines as activating ligands have, in combination with transition metals, played an important role in the development of sustainable catalytic solutions for academia as well as industrial applications. Caged phosphines are a class of phosphines possessing three-dimensional scaffolds and capable of providing unique control over steric and electronic properties. The versatility of the caged phosphine ligands has been demonstrated elegantly by the groups of Verkade, Gonzalvi as well as Stradiotto.¹ Our contribution to this area comes in the form of the 1,3,5-triaza-7-phosphaadamantane-based caged ligands, especially PTABS (KapdiPhos) that has proved to be a revelation in promoting heteroarene functionalization in a highly efficient way. The talk will therefore be centered around the journey from the development of the ligand to the varied applications including scale-up possibilities, eventually culminating into its commercialization.² New catalytic reactivity and its mechanism has been explored along the way and will also be discussed.



References

- 1. H. Shet, U. Parmar, S. Bhilare, A. R. Kapdi, Org. Chem. Front., 2021, 8, 1599-1656.
- a) S. Murthy Bandaru, S. Bhilare, N. Chryosochos, V. Gayakhe, I. Trentin, C. Schulzke, A. R. Kapdi, Org. Lett., 2018, 20, 473-476. b) S. Bhilare, S. MuthryBandaru, J. Shah, N. Chrysochos, C. Schulzke, Y. S. Sanghvi, A. R. Kapdi, J. Org. Chem., 2018, 83, 13088-13102. c) H. Shet, S. Bhilare, Y. S. Sanghvi, A. R. Kapdi, Molecules, 2020, 25, 1645. d) S. Bhilare, S. Murthy Bandaru, C. Schulzke, A. R. Kapdi, Chem. Rec., 2021, 21, 188-203. e) A. R. Kapdi, R. Sahu, Synlett, 2022, 34, 912-930 (account on KapdiPhos).



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Anant Kapdi was born in Mumbai, Maharashtra, India, in 1980, and studied chemistry at the University of Mumbai (MSc 2002) and York (MSc 2005; Dr. Ian J. S. Fairlamb). He completed his PhD in 2008 under the supervision of Dr. Fairlamb at The University of York (UK), before starting postdoctoral work in the research group of Prof. Lutz Ackermann at the Georg-August-University Gottingen as an Alexander von Humboldt Fellow. He returned to India in 2010 and was appointed as DST-SERC Fast Track Fellow (2011) and DST Inspire Faculty (2012) at the Institute of Chemical Technology, Mumbai before taking up UGC-FRP Assistant Professor position (2014) at the same institute. He has performed very well in his field of research, publishing more than 90 research publication in various reputed international journals and has 4 edited books in his name. He also has served as an Associate Editor of the Royal Society of Chemistry journal, RSC Advances. Recently, he was also elected as the Fellow of RSC under the Leader in Field category. He has also served as the founding Deputy Director of ICT-IOC Bhubaneswar off-campus of the Institute of Chemical Technology, Mumbai (2018-19). Anant has also been instrumental in the formation of India's first of kind Scientific consortium (Innovation Sustainability Chemistry Consortium-ISSC) and is currently the founding Coordinator (India). Currently he has been appointed as the Central Placement Coordinator for ICT, Mumbai and looks after the training and placement for all the 3 campuses of ICT. Anant has received many recognitions for his scientific contributions as well as the extensive administrative and outreach activities such as C. B. Murarka Best Assistant Professor Award 2018-19, Wellcome Trust/DBT India Alliance Early Career Fellow for 2021, DAAD Fellowship for Scientists (not availed), Alexander von Humboldt Return Fellowship (2013), Prof. N. R. Kamath Book Award.



IL-5

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Catalysis for sustainable and circular chemistry

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Achieving more sustainable chemical processes and enabling a circular economy are major goals of chemical research, which play a significant role in the implementation of resource- and cost-efficient chemical industry and advancement of society in terms of health, energy and environment. In this regard, the valorization of more abundant feedstocks, renewable resources and waste-materials to produce value-added products is of prime importance. In order to achieve these goals, the development and applicability of suitable catalytic processes is crucial. The major challenge in catalysis is to create 'ideal' catalysts which should be more stable and easily recyclable as well as highly selective and active. We are dealing on how to combine both homogeneous and heterogeneous catalysis aspects to create such ideal catalytic systems, especially based on nanoparticles (NPs) and single atoms (SACs) for advanced organic synthesis. Consequently, in the talk the design and catalytic applications of specific NPs and SACs as well as molecularly defined complexes for sustainable synthesis of essential fine and bulk chemicals as well as molecules used in life science applications will be presented. Next, catalytic applications on the valorization of renewable feedstocks (biomass and CO2) and recycling/upscaling of waste-plastics for enabling sustainable and circular chemistry will be discussed.

References

- V. G. Chandrashekhar, W. Baumann, M. Beller and R. V. Jagadeesh, *Science*, 2022, 376, 1433.
- R. V. Jagadeesh, K. Murugesan, A. S. Alshammari, H. Neumann, M.-M. Pohl, J. Radnik and M. Beller, *Science*, 2017, 358, 326.
- 3. R. V. Jagadeesh, A. E. Surkus, H. Junge, M. M. Pohl, J. Radnik, J. Rabeah, H. Huan, V. Schünemann, A. Brückner and M. Beller, *Science*, 2013, **342**, 1073.
- V. G. Chandrashekhar, T. Senthamarai, R. G. Kadam, O. Malina, J. Kašlík, R. Zbořil, M. B. Gawande, R. V. Jagadeesh and M. Beller, *Nature Catal.* 2022, 5, 20.
- 5. K. Murugesan, Z. Wei, V. G. Chandrashekhar, H. Neumann, A. Spannenberg, H. Jiao, M. Beller and R. V. Jagadeesh, *Nature Commun.*, 2019, **10**, 5443.
- B. Zhou, V. Chandrashekhar, Z. Ma, C. Kreyenschulte, S. Bartling, H. Lund, M. Beller and R. V. Jagadeesh, *Angew. Chem. Int. Ed.*, 2023, 62, e20221569.



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Jagadeesh was born on 2nd December 1979 and raised in Karnataka, India. He obtained PhD (2006) in Chemistry from Bangalore University, India under the supervision of Prof. Puttaswamy. After having performed Postdoctoral Research (2006-2008) in the group of Prof. David E. Richardson at the University of Florida, USA and worked few months as Assistant Professor (2009-2010) at VIT University, India he joined Leibniz Institute for Catalysis (LIKAT), Germany in the year 2010, where he currently is a Group Leader for Catalysis for Sustainable Syntheses. In Leibniz Institute for Catalysis, initially he has joined as a Scientist in the Department of Prof. Matthias Beller and then he became Group Leader at LIKAT first for Synergy between Homogeneous and Heterogeneous Catalysis and later for Catalysis for Sustainable Syntheses. He has obtained habilitation from the University of Rostock. He is also a Visiting Professor at VSB-Technical University of Ostrava, Czech Republic as well as Corporate Advisor and Visiting Professor at REVA University, Bangalore India. His research group works on sustainable catalytic processes for the synthesis of essential fine and bulk chemicals, pharmaceuticals and agrochemicals as well as for the valorization of renewable feedstocks (biomass and CO2) and circular chemistry for enabling circular economy (valorization of wastematerials, plastics-waste and use them as resources/feedstocks for chemicals upgrading). Important works of his group have been published in notable journals: 3 research papers in Science, >10 research papers in Nature Publishing Journals and 2 research papers in Cell-Press Journals. Interestingly, one work related to the development of iron-based nanocatalysts for an industrially important hydrogenation process has been highlighted and featured on the 'Cover of Science'. In addition, key works are highlighted in Science, Nature, Chemical & Engineering News (C&EN) and Chemistry World.



IL-6

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Polymer Nanoreactors for Aqueous Biphasic Catalysis

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Catalyst recovery and recycling is one very important aspect of the application of catalytic technology, with a strong impact on energy efficiency, industrial economy, and the environment (waste production). We will present a new approach for efficient biphasic catalysis using water to confine the catalyst, based on the catalyst covalent linking to the hydrophobic core of well-defined amphiphilic nanosized core-shell polymers. These polymers (see Figure below) have been efficiently synthesized by RAFT polymerization in aqueous dispersion.^{1a} Coordination of many different metals on the triphenylphosphine functions in the core has been achieved. Metal-containing core-shell functionalized polymers were efficiently used in the rhodium-catalyzed hydroformylation¹ and hydrogenation² of alkenes under aqueous biphasic conditions The catalyst could be recycled several times by simple decantation with low Rh leaching.



The results on the optimization of the nanoreactor's cores and the synthesis and the use of metal nanoparticles embedded into the core of nanoreactors in catalysis will be presented.³

References

- (a) X. Zhang, A. F. Cardozo, S. Chen, W. Zhang, C. Julcour, M. Lansalot, J.-F. Blanco, F. Gayet, H. Delmas, B. Charleux, E. Manoury, F. D'Agosto, R. Poli, *Chem. E. J.*, 2014, 15505 (b) A. F. Cardozo, C. Julcour, L. Barthe, J.-F. Blanco, S. Chen, F. Gayet, E. Manoury, W. Zhang, M. Lansalot, F. D'Agosto, R. Poli, H. Delmas, *J. Catal.*, 2015, **324**, 1.
- A. Joumaa, S. Chen, S. Vincendeau, F. Gayet, R. Poli, E. Manoury, *Mol. Cat.* 2017, 438, 267.
- (a) H. Wang, L. Vendrame, C. Fliedel, S. Chen, F. Gayet, F. D'Agosto, M. Lansalot,
 E. Manoury, R. Poli, *Chem. Eur. J.*, 2021, **27**, 5205. (b) H. Wang, A. M. Fiore, C.
 Fliedel, E. Manoury, K. Philippot, M. M. Dell'Anna, P. Mastrorilli, R. Poli, *Nanoscale Adv.*, 2021, **3**, 2554.



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Eric Manoury is a former student of the "Ecole Normale Supérieure de Cachan and he is currently a CNRS First Class Research Director at the Laboratoire de Chimie de Coordination (LCC) in Toulouse, France. After a PhD in Paris VI, Orsay under the supervision of Professor G.G.A. Balavoine dealing with chiral perborates for asymmetric epoxidation of alkenes and a post-doctoral stay with Professor K. Barry Sharpless at MIT working on the asymmetric hydroxylation of alkenes, he joined CNRS in 1993 in Orsay first and then in LCC in Toulouse. Since 2010, he is coleader of the team "Ligands, Complex Architectures and Catalysis" in the LCC. Since 2018, he is LCC Deputy Director. His main research interests are: Ferrocene Chemistry; Development of Chiral Ligands; Asymmetric Catalysis; Oxidation Catalysis; Asymmetric Hydrogenation; Asymmetric Coupling Reactions; Biphasic Catalysis with Polymeric Nanoreactors, Control Radical Polymerization.



10-13 December 2023

Green Chemistry and Heterogeneous Catalysis to Achieve Sustainable Development Goals

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Energy crisis and environmental deterioration has emerged as major problems around the world in recent times, mainly due to combustion of fossil fuels and their depletion. The utilization of solar energy to produce chemical fuels is an attractive and major strategy to address the global energy crisis and other environmental issues. Our research group has recently developed several nanostructured photocatalysts based on semiconductors, plasmonic materials, perovskites and upconversion nanoparticles, which can utilize the full solar spectrum from ultraviolet to infrared regions for energy generation and environmental remediation applications. In addition to photocatalytic hydrogen generation, nitrogen fixation and pollutants degradation, our group has also utilized these materials for biomass conversion, carbon dioxide reduction and Green organic transformations, either by functionalization or doping with a heteroatom. The highlights of the ongoing research work of our group will be presented.



References

- (1) V. Krishnan et al., Small 2023, 19, 2207053.
- (2) V. Krishnan et al., Fuel 2023, 341, 127713.
- (3) V. Krishnan et al., ACS Appl. Mater. Interfaces 2023, 15, 9412-9420
- (4) V. Krishnan et al., Chem. Eng. J. 2022, 431, 133695.
- (5) V. Krishnan et al., Green Chem. 2022, 24, 898-910.
- (6) V. Krishnan et al., Adv. Func. Mater. 2021, 31, 2009807.



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Prof. Venkata Krishnan completed his Ph.D. in Chemistry in 2006 from University of Stuttgart, Germany after completing his B.Sc. and M.Sc. degrees from PSG College of Technology, Coimbatore, Tamil Nadu, India. Subsequently, he worked as a postdoctoral researcher at University of Pennsylvania, U.S.A. from 2006 to 2010 and then as a research associate at National Institute for Materials Science (NIMS), Tsukuba, Japan from 2010 to 2012. He joined as a faculty at the Indian Institute of Technology (IIT) Mandi in April 2012 and is currently a full professor. His research group is mainly working in the field of Green Chemistry and Heterogeneous Catalysis for Energy and Environment Applications. He has successfully guided 11 Ph.D. and 26 M.Sc. students and is currently guiding 6 Ph.D. and 5 M.Sc. students, in addition to several short-term research interns. He has published more than 175 articles in well reputed international journals and is also a reviewer for several scientific journals. He has been bestowed with several awards, including DST INSPIRE faculty award, IIT Mandi foundation day award for excellence in teaching, MANA research fellowship, DoE postdoctoral fellowship, DFG doctoral fellowship, DAAD visiting scholar fellowship, etc. In addition to teaching and research, he has also served IIT Mandi in various administrative positions, such as first warden of the hostel in main campus, founding coordinator of Advanced Materials Research Center (AMRC), Associate Dean Research and most recently as Dean of Sponsored Research, Industrial Consultancy and International Relations (SRIC & IR), Director of IIT Mandi Catalyst (a technology business incubator) and Director of IIT Mandi iHub and HCI foundation (a technology innovation hub). Apart from academics, he likes reading books and is interested in linguistics.



10-13 December 2023

Redox Modulator Iron Complexes Triggering Apoptosis in Cancer Cells

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Iron regulatory proteins, including transferrin, employ overloaded iron pools in cancer cells to coordinate energy metabolism and redox homeostasis. Targeting the redox capacity of iron stores is a potential therapeutic modality to suppress cancer progression. Here I present that nitrogen-based heterocyclic iron chelators (IITK4001 and IITK4002) or their pre-synthesized iron complexes (IITK4003 and IITK4004) efficiently prevent the proliferation of liver cancer cells (EC₅₀: 0.34 µM for IITK4003), including liver cancer 3D-spheroids. These iron complexes generate highly reactive Fe(IV)=O species and accumulate lipid peroxides to promote oxidative stress in cells that impair mitochondrial function and affect ATP synthesis. The activation of the intrinsic apoptosis pathway in cancer cells and leakage of cytochrome c from mitochondria activating caspase were characterized as the selective mechanisms of action for lead iron complexes. Further, the delivery of IITK4003 using a polymeric nanocarrier exhibited a four-fold (EC₅₀ < 0.12 μ M) enhancement in the overall antiproliferative activity. Broadly, leveraging the inherent iron overload in cancer cells to selectively promote apoptosis is an attractive strategy for developing iron-chelating ligands/ iron complex-based anticancer therapeutics.





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Dr Dharmaraja Allimuthu is a trained chemical biologist who is working at the interface of organic chemistry and cell biology. Dharma received his PhD from IISER-Pune (2015-2010; Prof Harinath Chakrapani) in medicinal chemistry and then undertook postdoctoral studies with Dr Drew Adams (School of Medicine, Case Western Reserve University, Ohio, USA; 2015-2018) on exploring neurodegenerative disease biology. Dharma Joined the IITK-Chemistry department in Dec-2018. Currently, Dharma's lab is working on developing small molecule-based covalent discovery drug platforms employing activity-based protein profiling and chemoproteomics to accelerate the drug discovery process. Dharma's lab majorly targets are cancer and antimicrobial resistance using small molecule therapeuticsx.



IL-7

10-13 December 2023

Switchable ring-opening/organometallic-radical polymerization: towards recyclable vinyl polymers

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High-tech applications in many areas such as medicine, pharmacology and aeronautics require well-defined synthetic (co)polymer materials, i.e. with controlled chain-length and composition, narrow dispersity and high chain-end fidelity. Metal-mediated polymerization techniques such as ring-opening polymerization (ROP) of cyclic monomers and controlled radical polymerization (ATRP and OMRP) of vinyl monomers achieved several breakthroughs in the area of precision polymer synthesis.¹ New challenges in this domain have emerged, especially due to environmental and societal pressure, such as the use of biobased (co)monomers (CO₂, lactide) and benign metals,² and the need to develop recyclable materials.³



The synthesis and characterization of a cobalt(III) carboxylate complex will be presented, along with its application as

unimolecular initiator and moderator for the organometallic-mediated radical polymerization (OMRP) of vinyl acetate and the ROP of lactones.⁴ Taking advantage of the latter performances, we realized an unprecedented switch of polymerization mechanism, from radical to ring-opening using a single catalyst and without chemical modification, to produce partially (bio)degradable/recyclable and valuable copolymers.⁵

References

1. (a) C. Fliedel and R. Poli, J. Organomet. Chem., 2019, 880, 241,

(b) C. Fliedel, S. Dagorne and E. Le Roux, *Metal Complexes as Catalysts/Moderators for Polymerization Reactions*, in *Comprehensive Coordination Chemistry III*, eds. E. C. Constable, G. Parkin, L. Que Jr, Elsevier, 2021, chapter 9.14, 410-464.

3. J. B. Young, R. W. Hughes, A. M. Tamura, L. S. Bailey, K. A. Stewart, and B. S. Sumerlin, *Chem.* DOI: 10.1016/j.chempr.2023.07.004.

4. M. Michelas, J.-C. Daran, A. Sournia-Saquet, C. Fliedel and R. Poli, *Dalton Trans.*, 2023, **52**, 6791.

5. M. Michelas, R. Poli and C. Fliedel, in preparation.

^{2.} Y. Wang, Y. Zhao, S. Zhu, X. Zhou, J. Xu, X. Xie and R. Poli, *Angew. Chem. Int. Ed.*, 2020, **59**, 5988.



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Rinaldo Poli obtained a Ph.D. degree in 1985 from Scuola Normale Superiore (Pisa, Italy) under Fausto Calderazzo, with one year also spent at Imperial College London with Geoffrey Wilkinson. After a 2-year post-doc with F. A. Cotton at Texas A&M University, he joined the faculty of the University of Maryland at College Park and rose the rank to Full Professor. In 1996, he moved to France, first to Dijon until 2003, and since then to his current position in Toulouse where he teaches at ENSIACET and leads a research group at the Laboratoire de Chimie de Coordination of CNRS. His research interests are in transition metal chemistry, spanning from structure-bonding-reactivity relationships and mechanistic studies, especially for open-shell organometallic compounds, to the application of metal complexes to catalysis and to controlled radical polymerization.



IL-8

10-13 December 2023

Alkene Functionalizations under Ligand-Enabled Au(I)/Au(III) Redox Catalysis

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The past decade has witnessed tremendous advancements in the field of Au(I)/Au(III) redox catalysis. The pioneering work by Zhang and Toste group revealed the role of external oxidants to overcome the high redox potential of Au(I)/Au(III) couple ($E^0 = +1.41$ V) and to facilitate two-electron redox cycle in gold catalysis (Scheme 1a).¹ Later, the Glorius group introduced the merged gold/photoredox strategy to circumvent the need for a stoichiometric oxidant in these processes.² Our group and others introduced ethynylbenziodoxolones (EBXs) for accessing redox gold catalysis which served a dual role as oxidant and alkyne surrogate thereby avoiding the need for external oxidants.³

All of the above strategies were not amenable to the use of aryl halides, and thus their use in gold-catalyzed cross-coupling reactions remains forbidden. In recent years, ligand-enabled gold-catalyzed organic reactions have emerged as a valuable tool, allowing for the use of aryl halides as cross-coupling partners. In this talk, I will discuss our most recent work in the area of alkene functionalization employing cross-coupling reactivities.^{4,5,6,7}

Scheme 1. Concept of Ligand-Enabled Enantioselective Redox Gold Catalysis



References:

- 1. Review: J. Miro; C. del Pozo, Chem. Rev. 2016, 116, 11924.
- 2. Review: M. N. Hopkinson; A. Tlahuext-Aca; F. Glorius, Acc. Chem. Res. 2016, 49, 2261.
- 3. Review: S. Banerjee; V. W. Bhoyare; N. T. Patil, Chem. Commun. 2020, 56, 2677.
- 4. C. C. Chintawar, A. K. Yadav, N. T. Patil, Angew. Chem. Int. Ed. 2020, 59, 11808.
- 5. M. V. Mane; N. T. Patil, J. Am. Chem. Soc., 2022, 144, 7089.
- 6. A. G. Tathe, Urvashi, A. K. Yadav, C. C. Chintawar, N. T. Patil, ACS Catal. 2021, 11, 4576.
- 7. V. W. Bhoyare, E. Daiann Sosa Carrizo, C. C. Chintawar, V. Gandon, N. T. Patil J. Am. Chem. Soc. 2023, 145, 8810.



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Dr. Patil's broad research interests include the development of metal-, organo- and organo/metal-catalyzed enantioselective methods as well as total synthesis of natural products. He has been the recipient of the CNR Rao National Prize for Chemical Sciences, SERB Distinguished Investigator Award, CRSI Bronze Medal, INSA Young Scientist Medal, Alkyl Amines – ICT Foundation Day Young Scientist Award and Avra Young Scientist Award. He has also served as "Young Associate" of the Indian Academy of Sciences, Bangalore during 2010-2013. Recently, he was elected as Fellow of the Indian National Science Academy (FNA), Fellow of The National Academy of Sciences (FNASc), Fellow of Maharashtra Academy of Sciences (FMASc) and fellow of The Royal Society of Chemistry (FRSC).



IL-9

10-13 December 2023

Rhodium complexes with planar-chiral cyclopentadienyl ligands as catalysts for regio- and stereo-selective C-H activation reactions

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Various rhodium catalysts with planar-chiral cyclopentadienyl ligands can be assembled in one or two steps from the commercially available [(cod)RhCl]₂ and *tert*-butyl-acetylene [1,2]. Pure enantiomers of these complexes were obtained by crystallization or chromatographic separation of their diastereomeric adducts with L-proline or L-phenylglycinol. The resolved complexes catalyze C-H activation and annulation of arylhydroxamates with alkenes giving valuable dihydroisoquinolones in excellent yields with high regio- and stereoselectivity (>90% ee). Critical analysis revealed that noble metals, such as rhodium, typically contribute less than 10% to the total cost of fine organic synthesis and their replacement by 3d metals can in fact make catalytic reactions more expensive and less sustainable [3].



70-90%, >90%ee

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References

1. E. A. Trifonova, N. M. Ankudinov, A. A. Mikhaylov, D. A. Chusov, Y. V. Nelyubina, D. S. Perekalin, *Angew. Chem. Int. Ed.* 2018, **57**, 7714.

2. A. V. Kolos, Y. V. Nelyubina, B. Sundararaju, D. S. Perekalin, *Organometallics* 2021, **40**, 3712.

3. A. A. Komarova, D. S. Perekalin, Organometallics 2023, 42, 1433.



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Dmitry Perekalin was born in Moscow, Russia and received his Ph.D. degree in Organometallic Chemistry at A.N. Nesmeyanov Institute of Organoelement Compounds (INEOS RAS) in 2005. He then worked as a visiting researcher at the Institute of Inorganic Chemistry of the Czech Academy of Sciences (laboratory of Prof. Bohumil Štíbr), the Heriot-Watt University of Edinburg (laboratory of Prof. Alan J. Welch), and the University of Rennes (laboratory of Prof. Pierre Dixneuf). He was appointed as a senior research fellow at INEOS RAS in 2010 and became the head of the lab in 2019. His scientific interests are focused on the synthesis of transition metal pi-complexes and their application in catalysis, photochemistry, and biochemistry. Outside of work he enjoys playing chess, archery and hiking.



IL-10

10-13 December 2023

Site selectivity in ruthenium-catalyzed C-H bond activation around cyclic amides

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Selective C–H functionalization for the formation of new C-C and C-heteroatom bonds is of great importance in current organic synthesis and in late-stage transformations of functional target molecules. The strategy based on transition metal-catalyzed directed C-H activation has found many applications with various types of directing groups. We present here applications of ruthenium catalysts in arylation,¹ alkylation,² alkenylation,³ hydroxylation,⁴ benzoxylation⁵ and amidation⁶ of cyclic amides and imides featuring two possible reactive sites for C-H activation (Figure 1). The high site- and regio-selectivities of these reactions will be emphasized.



Figure 1. Two possible sites for C-H activation in N-arylisoindolinone and N-arylphthalimide

References

- 1. Y. -C. Yuan, C. Bruneau, T. Roisnel, R. Gramage-Doria, *J. Org. Chem.*, 2019, **84**, 12893-12903.
- Y. -C. Yuan, M. Goujon, C. Bruneau, T. Roisnel, R. Gramage-Doria, J. Org. Chem., 2019, 84, 16183-16191.
- 3. Y. -C. Yuan, C. Bruneau, T. Roisnel, R. Gramage-Doria, *Catal. Sci. Technol.*, 2019, **9**, 4711-4717.
- Y. -C. Yuan, C. Bruneau, V. Dorcet, T. Roisnel, R. Gramage-Doria, J. Org. Chem., 2019, 84, 1898-1907.
- 5. Y. -C. Yuan, C. Bruneau, T. Roisnel, R. Gramage-Doria, *Org. Biomol. Chem.*, 2019, **17**, 7517-7525.
- 6. Y. -C. Yuan, Q. -L. Lu, X. -T. Zhu, S. Posada-Pérez, M. Solà, A. Poater, T. Roisnel, R. Gramage-Doria, *Org. Chem. Front.*, 2023, **10**, 42-53.



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Dr. Christian Bruneau graduated in chemistry from the Institut National Supérieur de Chimie Industrielle de Rouen (France, 1974) and got his PhD at the University of Rennes (1979). He obtained a CNRS position in 1980 where he initially worked on environmental chemistry, and since 1986 has been working in the field of transition metal catalysis at the University of Rennes. Since 2017, he is Emeritus researcher at the University of Rennes.

He has been mainly involved in ruthenium and recently iridium-catalyzed selective transformations (additions to terminal alkynes, olefin metathesis, allylation, sp^2 and sp^3C-H bond activation and functionalization, hydrogen transfer, asymmetric catalysis, bio-resources transformations) with a focus on green and sustainable catalysis.

From 2000 to 2011, he has been the head of the CNRS-University of Rennes research group "*Organometallics and Catalysis*" at the Institute of Chemical Sciences in Rennes.

He has published 375 papers in scientific journals including 34 book chapters and 27 review articles, and he is co-editor of 3 books. He is the recipient of the prize of the Coordination Chemistry Division (2008) and Le Bel prize (2016) from the French Chemical Society, and Paul Langevin prize (2012) from the French Academy of Sciences.



IL-11

10-13 December 2023

Plasmonic Black Gold: Harnessing Hot Electrons for Solar Energy Harvesting and Catalysis

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Capture and then conversion of CO₂ to valuable chemicals and fuels is the crucial challenge for Circular Economy. In this regard, we discovered a new nanosilica, Dendritic Fibrous Nano-Silica (DFNS),^{1,2} and reported several applications of DFNS for catalysis and CO₂ capture-conversions, such as Black Gold³, Defective Catalysts^{4,5}, Solid Acids⁶, Lithium Silicates Nanosheets⁷ and Magnesium⁸. In this talk, I will discuss one of our recent discoveries for solar energy harvesting and CO₂ utilization, using the concept of "Black Gold as an Artificial Tree". We transformed yellow gold into black gold by changing the size and gaps between gold nanoparticles supported on DFNS.³ Black gold harvest board band light of the solar spectrum, the entire visible region, as well as in the near-infrared region. We have then designed and synthesized nickel-laden black gold catalysts, with a very high photocatalytic CO production rate and 95 % selectivity.⁹ The catalyst was stable for at least 100 h. Black Gold-Ni also catalyzes several other challenging reactions, such as H₂ dissociation, C-Cl bond activation, and propene & acetylene hydrogenation, using visible light at room temperature, a perfect example of green catalysis. I will also briefly talk about plasmonic thin films of nickel nitride as photocatalysts.¹⁰

References

- 1. V. Polshettiwar, Acc. Chem. Res., 55, 1395 (2022).
- 2. A. Maity, R. Belgamwar, V. Polshettiwar Nature Protocol, 14, 2177 (2019).
- 3. M. Dhiman, A. Maity, A, Das, R. Belgamwar, B. Chalke, Y. Lee, K. Sim, J. M. Nam, V. Polshettiwar, *Chemical Science* **10**, *6694* (2019).
- 4. A. K. Mishra, R. Belgamwar, R. Jana, A. Datta, V. Polshettiwar, *Proc. Natl. Acad. Sci.* U.S.A **117**, 6383 (2020).
- 5. R. Belgamwar, R. Verma, T. Das, S. Chakraborty, P. Sarawade, V. Polshettiwar, *J. Am. Chem. Soc.* **145**, 8634 (2023).
- 6. A. Maity, S. Chaudhari, J. J. Titman, V. Polshettiwar, Nature Comm. 11, 3828 (2020).
- R. Belgamwar, A. Maity, T. Das, S. Chakraborty, C. P. Vinod, V. Polshettiwar, *Chemical Science*, 12, 4825 (2021).
- 8. S. A. Rawool, R. Belgamwar, R. Jana, A. Maity, A. Bhumla, N. Yigit, A. Datta, G. Rupprechter, V. Polshettiwar, *Chemical Science*, **12**, 5774 (2021).
- R. Verma, R. Belgamwar, P. Chatterjee, R. B. Vadell, J. Sá, V. Polshettiwar, ACS Nano, 17, 4526 (2023).
- S. Singh, R. Verma, N. Kaul, J. Sa, A. Punjal, S. Prabhu, V. Polshettiwar, *Nature Comm.* 14, 2551 (2023).



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Prof. Vivek Polshettiwar, after his Ph.D. in 2005, worked as

a postdoc in France and USA for a few years before starting his own independent group at KAUST in 2009. In 2013, he moved to TIFR, and his group is working on the development of novel nanomaterials as catalysts to combat "climate change". Nanocatalysis can help design catalysts with excellent activity, greater selectivity, and high stability. Their properties can easily be tuned by tailoring the size, shape, and morphology as well as defects and interfaces of the particular nanomaterial. He has published nearly 120 articles with an h-index 62 and around 16000 citations in reputed journals like PNAS, JACS, Nature Communications, Nature Protocol, AngewChem, Chem. Sci., ACS Nano, ACS Catalysis, etc. He also filed 12 national and international patent/patent applications.

He is the recipient of the prestigious ORISE Research Fellowship at US-EPA. He was awarded as Top-25 cited author in 2011 by Tetrahedron and Young Scientist Award at DSL-2012. He also received an Asian Rising Star lectureship at 15th Asian Chemical Congress (ACC), Singapore (2013), from Nobel Laureate Professor Ei-ichi Negishi. In 2015, he was admitted as a Fellow of the Royal Society of Chemistry (RSC), United Kingdom. He was awarded a Bronze medal by the Chemical Research Society of India (CRSI), India. He was awarded the prestigious Materials Research Society of India - MRSI Medal 2019. He was elected a Fellow Maharashtra Academy of Sciences in 2019. In 2020, he received Young Research Award in Nano Science & Technology from the Department of Science & Technology (DST), Gov. of India. In 2021, he was elected as a Fellow National Academy of Sciences, India (NASI). Vivek received the 2022 IUPAC-CHEMRAWN VII prize for green chemistry from IUPAC and National Prize for Research on Environmental Chemistry. In 2023, he received the Falling Walls Award in Physical Sciences.



IL-12

10-13 December 2023

Sustainable Chemistry from Renewable Resources – The strategy of Solvay

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As an industrial group committed to sustainable development, Solvay is committed to finding new differentiating products and solutions for our customers. Decreasing our energy, carbon and CO₂ footprints is our global ambition. As a chemist, developing new products coming from renewable resources is also a clear target. However, this should always be performed integrating life cycle analysis including the applications to ensure that high quality solutions for our customers are provided. Today we are accelerating these developments with the launch in May 2022 of our fourth growth platform dedicated to renewable materials and biotechnology.

After a short presentation of our group and our growth platform, the topic will be illustrated with a few selected examples of sustainable chemistry developed from renewable resources.

References

1. P. Marion, B. Bernela, A. Piccirilli, B. Estrine, N. Patouillard, J. Guilbot and F. Jérôme, *Green Chem*istry, 2017, **19**, 4973-4989

2. S. Charati, C. Cochennec, M. Dahanayake, P. Gilbeau, M. P. Labeau, P. Lapersonne, P. Marion, S. Martins, F. Monnet, R. Nascimento, *Chemicals and Fuels from Bio-Based Building Blocks,* Editors Cavani, Albonetti, Basile & Gandini, Wiley, 2016, **2**, chap. 24, 615-641.

3. I. Scodeller, S. Mansouri, D. Morvan, E. Muller, K. de Oliveira-Vigier, R. Wischert, F. Jérôme, *Angew. Chemie Int. Ed.*, 2018, **57** (33), 10510-10514.



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Philippe Marion graduated from the National Chemistry School of Montpellier in 1987 and received his PhD degree in organic chemistry and heterogeneous catalysis from Lyon University in 1990 under the supervision of Dr M. Joucla and Dr J. Jenck in a joint lab between Rhone Poulenc and CNRS. Hired by Rhone-Poulenc where he held different positions as researcher then project, team, group and department managers always within Rhone Poulenc, Rhodia then Solvay.

His research has driven the development of many different products and processes in the field of intermediates, specialty chemicals and performance products. He has coauthored around 30 international publications and book chapters and around 100 families of patents. He is today Fellow scientist and advisor of main catalysis and organic chemistry developments within Solvay. He is also senior distinguished fellow of the French Chemical Society since 2022.



SL-3

10-13 December 2023

Selective Methane Oxidation to Acetic Acid using Molecular Oxygen over a Metal-Organic Framework-Supported Copper Catalyst

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Acetic acid is an industrially important chemical, produced mainly via carbonylation of methanol using precious metal-based homogeneous catalysts. As a low-cost feedstock, methane is commercially transformed to acetic acid via a multi-step process involving energy-intensive methane steam reforming, methanol synthesis, and subsequently, methanol carbonylation. We have developed a direct single-step conversion of methane to acetic acid using molecular oxygen (O_2) as the oxidant under mild conditions over a mono-copper hydroxyl site confined in a porous metal-organic framework (MOF). The heterogeneous MOF-supported single-site copper hydroxyl catalyst gave exceptionally high acetic acid productivity of 335 mmolg_{cat}⁻¹ in 100% selectivity at 115 °C in water. Our spectroscopic and theoretical studies and controlled experiments reveal that the conversion of methane to acetic acid occurs via oxidative carbonylation, where methane is first activated at the copper-hydroxyl site via σ -bond metathesis to give Cu-methyl species followed by carbonylation with in-situ generated carbon monoxide and subsequent hydrolysis by water. We demonstrate that the confinement of an active monocopper hydroxyl site within a porous MOF represents an efficient strategy to develop novel earth-abundant metal catalysts for the selective functionalization of methane and other light hydrocarbons. This work may guide the rational design of heterogeneous abundant-metal catalysts to activate and convert methane to acetic acid and other valuable chemicals under mild and environment-friendly reaction conditions.



References

N. Antil, M. Chauhan, N. Akhtar, R. Newar, W. Begum, J. Malik, K. Manna, ACS Catalysis, 2022, **12**, 11159-11168.
 N. Antil, M. Chauhan, N. Akhtar, R. Kalita, K. Manna, J. Am. Chem. Soc., 2023, **145**, 6156-6165.



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Kuntal Manna is an Associate Professor in the Department of Chemistry of Indian Institute of Technology Delhi (IIT Delhi), India. He completed his master's in Chemistry from IIT Kanpur in 2006. After receiving his PhD in Inorganic Chemistry from Iowa State University in 2012 under the guidance of Prof. Aaron D Sadow, Dr. Manna was a postdoctoral researcher at the University of Chicago (2013-2016). He joined the Department of Chemistry of IIT Delhi as an Assistant Professor in 2017. His research focuses on developing heterogeneous catalysts for sustainable organic transformations, functionalization and upgradation of light hydrocarbons, and energyrelated transformations.



SL-4

10-13 December 2023

CIRCULAR FOAM: Chemical Recycling of Rigid Polyurethane Foams

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Reducing energy consumption is the best way to reduce greenhouse gas emissions. Rigid polyurethane (PU) foam is a material with excellent insulating properties that has made a significant contribution to reducing greenhouse gas emissions in the cold chain and in the construction industry for decades. At the end of its life, however, rigid PU foam is nowadays either disposed of in landfills or recycled energetically via incineration. The EU project CIRCULAR FOAM aims to develop a closed-loop circular ecosystem for end-of-life (EoL) rigid PU foam to demonstrate that such insulation materials are recyclable.¹

Here we focus on the development of a new closed-loop chemical recycling methodology for the re-use of PU rigid foam. The primary aim is the recovery of both a re-polyol and a re-amine (as precursor for re-pMDI, the polymeric isocyanate used for the production of PU rigid foams) via selective catalytic cleavage of urethane bonds. Here we present two different chemical recycling technologies, namely chemolysis and catalytic pyrolysis, also called "smart" pyrolysis. In the case of smart pyrolysis, the goal is to produce aniline, the precursor to pMDA. Consequently, the development of efficient catalytic methods, downstream product separation, evaluation of re-PU materials with respect to techno-economic analysis and life-cycle assessment are all integral parts of the CIRCULAR FOAM project.



Figure 1: chemical recycling of PU rigid foam via chemolysis and smart pyrolysis

References 1. https://circular-foam.eu/



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Suresh Raju was born in a small village in Karur (Tamilnadu), India. After chemistry studies at St. Joseph's College affiliated to Bharathidasan University in Tiruchirappalli, he received EGIDE scholarship in 2009 for the international Master program in catalysis and green chemistry at the University of Rennes 1 in France. In 2015, he completed his PhD in organometallics and catalysis under the guidance of Prof. Bert Klein Gebbink at Utrecht University, Netherlands. Afterwards, he moved to Germany by receiving the Goettingen International short-term postdoctoral fellowship in the group of Prof. Sven Schneider at the University of Goettingen. Since 2018, Suresh is associated with the CAT Catalytic Center Aachen (joint R&D Center of RWTH Aachen University and Covestro) in various roles as scientist, team leader and project leader. His recent research activities involve catalytic process developments for CO_2/CO conversion, circular economy, and innovative chemical recycling technologies for polyurethanes.



IL-13

10-13 December 2023

Catalysis for C-C and C-heteroatom bond-forming reactions

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Catalytic C-C and C-heteroatom bond-forming reactions represent key transformations for the synthesis of valuable products or advanced intermediates. This presentation will highlight our recent efforts toward developing new and sustainable metal-catalyzed and metal-free C-H functionalizations and functional group interconversions. In particular, light-mediated metal-, photo-, electro- and mechanocatalyzed transformations will be presented.



10-13 December 2023

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Magnus Rueping studied at the Technical University of Berlin, Trinity College Dublin and ETH Zürich, where he completed his diploma thesis under the direction of Professor Dieter Seebach. He stayed in the Seebach group and obtained his Ph.D. from the ETH in 2002 working on the synthesis, the structural and the biological aspects of oligo(hydroxybutanoates) and of β - and γ -peptides. Magnus then moved to Harvard University to work with Professor David Evans on enantioselective transition-metal catalysis.

In August 2004, he was directly appointed to a C3-professorship, the Degussa Endowed Professorship of Synthetic Organic Chemistry at Johann Wolfgang Goethe University of Frankfurt. After four years in Frankfurt, Magnus received several offers of academic positions and decided to accept a Chair and Full Professorship at RWTH Aachen University and since 2016 he is Professor of Chemical Science and member of the KAUST Catalysis Center.

His group's research activities are directed toward the development and simplification of catalytic methodology and technology, and their application in the sustainable synthesis of diverse functional molecules. Over the years the group has developed new catalysts and catalytic concepts involving various types of catalysis: homogeneous and heterogeneous catalysis, asymmetric catalysis, metal catalysis, organocatalysis and biocatalysis, photo(redox) catalysis, electrocatalysis, mechanocatalysis as well as combined processes resulting in tandem or cascade procedures and applications. In addition, the group is involved in the development of continuous flow (micro)reactor systems, including feedback algorithms and inoperando analytics.



IL-14

10-13 December 2023

Role of catalysts to handle challenges of refineries in an era of energy transition.

Alex C Pulikottil^{*} and M Sau

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We are in an era of energy transition and the environment driven mandate is shaping a change in way the current day oil refining operations is done. Current day refineries that primarily focus on fuels production are looking at options to increase the petrochemical intensity in its operations. Process units needs to run at maximum efficiency, regulatory requirements for both product quality and environmental performance must be met. Along with there is a need to adapt and respond to changes in feedstock availability and product slate shifts required for profitable operation of a refinery. Oil refining has remained a catalyst intensive domain, wherein catalyst innovations and breakthrough has fuelled the growth of modern refining industry and the current scenario opens challenges and research opportunities in refining catalysis. Fit for purpose refining catalysts can be a drop in tool to align refinery to navigate the challenges of energy transition with goals for sustainability and the presentation will highlight this aspect.



10-13 December 2023

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Dr. Alex C Pulikottil leads the research vertical of Catalyst and Petrochemicals & Polymers at Research & Development Centre of Indian Oil Corporation Limited.

He holds a PhD from the Indian Institute of Technology, Madras and has over 25 year experience in downstream hydrocarbon sector, notably in refinery process and catalyst development. He is instrumental in development of several indigenous process technologies, indigenization of DHDS/DHDT catalyst and several FCC catalyst additives and their commercial deployment. He has to his credit 25 research publications and over 30 patents and is recipient of several awards including Petrofed (Petroleum Federation), CHT (Centre for High Technology) and FIPI (Federation of Indian petroleum Industries) awards.


IL-15

10-13 December 2023

Homogeneous supported catalysis for (industrial) applications in crosscoupling reactions

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The role of organometallic catalysis allowing the targeted production of high value-added products no longer needs to be demonstrated, but the fine chemicals sector dedicated to health applications remains very demanding for innovative and sustainable synthesis routes. In this context, obtaining minimal residual traces of metal in the target products is an important objective; Most transition metals are indeed toxic species, and their presence in valuable chemicals is accurately regulated, depending on their mode of administration. Additionally, residual amounts of metals can interfere with subsequent synthetic steps of the process.

Making valuable catalysts insoluble and therefore easy to remove, or even reuse, is an elegant way to answer the principles of green chemistry and sustainable development. Since cross-coupling reactions are prevalent tools in the fine chemical industry, we propose the synthesis and the evaluation of the catalytic activity of Pd–NHC complexes covalently grafted on calix[8]arene supports in the Suzuki-Miyaura and Buchwald-Hartwig reactions. The recent results obtained for both topics will be the subject of this presentation.



References

1. I. Abdellah, C. Martini, A. Dos Santos, D. Dragoe, V. Guérineau, V. Huc, E. Schulz, *ChemCatChem*, 2018, **10**, 4761.

2. S. Abi Fayssal, T. Naret, V. Huc, J. Buendia, C. Martini, E. Schulz, *Catal. Sci. Technol.*, 2021, **11**, 5223.

3. S. Abi Fayssal, T. Naret, J. Buendia, A. Labattut, V. Huc, C. Martini, E. Schulz, *Adv. Synth. Catal.*, 2022, **364**, 947.



10-13 December 2023

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Emmanuelle Schulz graduated from ESCIL in Lyon and received her Ph.D. degree in 1992 for studies concerning the total synthesis of Strigol (Pr. P. Welzel, Ruhr-Universität Bochum/Pr. J. Goré, Université de Lyon). After an industrial postdoc (Rhône-Poulenc Agrochimie), she joined the group of Prof. M. Lemaire in Lyon and obtained a permanent position at the CNRS. Since 2000, she has been working in the Institut de Chimie Moléculaire et des Matériaux d'Orsay (Université Paris-Saclay) and was nominated Directrice de Recherches CNRS in 2005. She was responsible for the Catalyse Moléculaire team between 2009 and 2019. Her research interests are mainly directed towards asymmetric catalysis and homogeneous supported catalysis (Orcid 0000-0002-0844-8825). She particularly explored the enantioselective hydroamination reaction promoted by chiral rare-earth based catalysts. New procedures for the easy recovery and reuse of (chiral) organometallic catalysts are also developed in her group. These methodologies imply the preparation of organic conducting metal-containing polymers by electrochemistry and their use as multipurpose asymmetric catalysts. Non covalent interactions such as those involved in charge transfer complexes are also exploited for the recovery of chiral catalysts. Finally, covalent grafting on organic platforms is also being studied for the immobilization of organometallic complexes that can be used for crosscoupling reactions on an industrial scale. Elected to the board of the Organic Chemistry Division of the French Chemical Society since 2018, she has been its president since July 2021.



IL-16

10-13 December 2023

Hydrogenation of some Bioplatform molecules over tailored polyoxometalates Prof. (Dr.) Anjali Patel

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Due to a shortage of natural sources, the gasoline blenders, fuel additives, flavouring agents and pharmaceutical industries meet the worldwide need for bio-based value-added products through carbonyl group containing bioplatform molecules [1]. Amongst, Furfural (FA) and Levulinic acid (LA) are most important bioplatform molecules, obtained from the lignocellulose and low-cost aldehyde, from which number of value-added products can be synthesized, especially by hydrogenation. In this direction to achieve the goal, generally precious metals such as Pd, Pt, Au based catalyst have been used to obtain single selectivity for the desired product and towards the same, however they are restricted to commercial use from economical viewpoint (low natural abundance and high cost) [2-3]. To overcome this, use/replacement of these precious metal is still a challenge. In this situation, bi-functional catalysts based on earth abundant transition metal exchanged supported polyoxometalates can be one of the best options as they combine the benefits of both transition metals and s heteropolyacids [4].



Scheme 1. Selective hydrogenation of FA and LA to value added products

In the present talk, the designing as well as the characterizations of bifunctional catalysts comprising Ni and 12-tungstophosphoric acid supported/anchored to Zeolite Y and neutral alumina will be described. The selectivity of the products obtained via hydrogenation of furfural and levulinic acid with 2-propanol and formic acid as internal hydrogen source will be discussed with respect to the different reaction conditions. The role of Ni as well as effect of the support will also be highlighted.

Reference

- M. Zhao, K. Yuan, Y. Wang, G. Li, J. Guo, L. Gu, W. Hu, H. Zhao, Z. Tang, Nature, 2016, 539, 76–80.
- 2. C.-C. Li, C.-H. Hsieh, Y.-C. Lin, Mol. Catal. 2022, 523, 111720.
- **3.**R. Nie, Y. Tao, Y. Nie, T. Lu, J. Wang, Y. Zhang, X. Lu, C.C. Xu, ACS Catal. 2021, 11, 3, 1071–1095.
- 4. J. Patel, A. Patel, Renew. Energ., 2022, 201, 190-201.



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Dr. Anjali Patel, working as a Professor (Inorganic Chemistry) since 2011 at the Department of Chemistry, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat. She worked as the Head of the Department and as the former joint director of BSc. Higher payment program, M.K. Amin Arts and Science College, Padra, Vadodara. Her research interest focuses on Polyoxometalates, Heterogeneous Catalysis, Green Chemistry and Materials. She has 150 papers in international journals including five review articles (Highest impact factor = 48.16), 3 patents, 6 book chapters and 2 books to her credit. She has visited various countries like USA, UK, China, France, Germany, Italy, Russia and Japan for delivering lectures/seminar at various international level as well as different societies. She also worked as a member in different committees such as WOS-A etc. She has been awarded the prestigious Fellow of the Royal Society of Chemistry (FRSC) and the Life fellow of Indian chemical society (FICS). She has been elected for the 7th Venus International Science and Technology Awards – VISTA 2021.



FL-1

10-13 December 2023

Transition-metal-catalyzed C(sp²)–H functionalization of Phthalazinones

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Transition-metal catalyzed C–C bond formation lies at the heart of synthetic organic chemistry as it creates sizable molecular diversity in carbocycles and heterocycles. In synergy with directing groups, transition-metal catalyzed C– H bond activation has extended the perimeter of several reactions and made groundbreaking strategies to access previously inaccessible molecular structures. Phthalazinone is an interesting N-heterocycles, and it is ubiquitously embodied in natural products, biologically active molecules, and pharmaceuticals. Owing to their intriguing structural architecture and versatile biological activities, phthalazinone synthesis has gained immense attention from synthetic and medicinal chemists. Our research group mainly focused on $C(sp^2)$ –H functionalization of phthalazinones catalyzed by ruthenium, cobalt, and palladium salts.

Phthalazinones: by ruthenium catalysis, alkylation and formylmethylation were achieved with maleimide/ethyl glyoxylate and vinylene carbonate respectively; by cobalt catalysis, chlorination was achieved using chloroform; and by low-loading palladium catalysis, cross-dehydrogenative *meta/para*-arylation was achieved under light with simple arenes.



References

1. C. Sivaraj, A. Ramkumar, N. Sankaran and T. Gandhi, Org. Biomol. Chem., 2021, 19, 8165.

2. A. Ramkumar, R. Sreedharan, P. Rajeshwaran and T. Gandhi, *Org. Biomol. Chem.*, 2023, **21**, 2695.



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Thirumanavelan Gandhi obtained his M.Sc. in Chemistry from Muthurangam Govt Arts College, Vellore in 1999 and his Ph.D. degree in Chemistry from Indian Institute of Science, Bangalore in 2005 under the guidance of Prof. Balaji R. Jagirdar. He did his postdoctoral research at The Johns Hopkins University, Baltimore with Prof. Kenneth D. Karlin for three years (2006-'08). He worked as a senior scientist in Alent plc, Bangalore for two years (2009-'11) before joining Vellore Institute of Technology, Vellore in 2011. He is a recipient of Young Scientist Award conferred by Chemical Research Society of India (CRSI). His research interests include the development of novel catalysts and their application towards C–H activation/functionalization.



FL-2

10-13 December 2023

Catalytic Dearomatisations (CRDs) to Visible Light Dearomatisations (VDRs)

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Dearomative transformations has grasped immense attention of chemists and in this context, **Dearomatization** of arenols is considered to be the shortest and most powerful approach towards the construction of a range of molecular architectures from simple planar starting materials. We have been working on *intra*- or *inter*- Dearomative transformations. The talk will represent our journey from Tribromide based dearomatisations to visible light dearomatization of arenes from natural resources as a powerful strategy for the generation of three-dimensional molecular architectures.



References

- 1. Bishi. S, Sarkar. D ChemSusChem 2023 (Just Accepted).
- 2. Roy. B; Kuila. P; Sarkar.D J. Org. Chem 2023, 88, 13, 7977-7987
- 3. Bera. N; Sarkar. D J. Org. Chem 2023, 88, 15, 10925-10945

4.Samanta. S; Sarkar. D Chem Photo Chem 2023 87,(Accepted Article) doi/abs/10.1002/cptc.202200335

- 5. Bera .N, Koenig. B, Sarkar. D J. Org. Chem 2022. 87, 21, 13529-13541
- 6. Sahoo. S; Sarkar. D J. Org. Chem 2022 87, 15, 9729-9754
- 7. Bera. N; Samanta. S; Sarkar. D J. Org. Chem 2021, 86, 23, 16369-16395
- 8. Rout. N; Sarkar. D Organic Letters 2019 21, 11, 4132-4136



10-13 December 2023

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Dr. Debayan Sarkar is presently an Associate Professor of Chemistry at the Indian Institute of Technology Indore (IIT Indore). Before this he worked as an Associate Professor in the Department of Chemistry at National Institute of Technology, Rourkela, Odisha, India. He has completed his M.Sc with Organic Chemistry specialisation from University of North Bengal (NBU) in the year 2005 followed by a Ph.D in Organic Synthesis from Indian Association For The Cultivation of Science (IACS) in the year 2011, Jadavpur Kolkata under the supervision of Prof. R. V.Venkateswaran in 2011. After that he travelled to carry out his post-doctoral studies at Stanford University (USA) under the mentorship of Prof. Barry M Trost (2012-2013). He was recently deputed as a Visiting Senior Assistant Professor at Graduate School of Pharmaceutical Sciences, Tohoku University (Japan) under the mentorship of Prof. M. Yamaguchi (Dec 2015- March 2016). He was at the University of Leipzig Germany as a DAAD Research Professor with Prof. Christoph Schneider (2018-2019). He worked with Prof. Burkhard Koenig at University of Regensburg Germany as an ICMR International Fellow from Jan-Dec 2020. He has been recipient of prestigious awards like SERB TETRA Award, RC Tripathy Research Excellence Award by Orissa Chemical Society, DST Inspire faculty award (2013), BRNS-DAE Young Scientist Award (2014), Indo-US Research Award (2012), DAAD Visiting Professor (2018). Research interest includes Visible Light Catalysis, Asymmetric Dearomatisation reactions, Atom Economic couplings, Complex total synthesis of natural products. He has 60 research publications in International Journals of Repute, 2 Patents and guided 6 Ph.D students and 12 Ph.d students are presently undergoing their doctoral studies under his supervision. Presently, he is also heading the Centre for Rural Development and Technology (CRDT) at IIT indore.



FL-3

10-13 December 2023

Heterogenous Non-noble Metal Catalysts for Transfer Hydrogenation of various Functional Group Derivatives

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Catalytic transfer hydrogenation of functional group derivatives is of keen interest for researchers involved in organic synthesis, as the resultant amines are extensively featured in natural products, drugs, agrochemicals, dyes, etc.¹ In contrast to the traditional reduction of various functional group derivatives using (over)stoichiometric reductants, the direct transfer hydrogenation process is more attractive owing to its sustainability approach. The liquid hydrogen carrier for transfer hydrogenation has received a great deal of attention from both academia and industry as an alternative to the traditional high-pressure-hydrogen process, due to its better efficiency, atom economy and sustainability features.² This presentation provides the status and insight into the recent progress made in catalytic transfer hydrogenation through liquid hydrogen carrier using novel Manganese and Palladium catalysts with various support materials that would efficiently perform the transfer hydrogenation and hydrogenolysis process of various functional group derivatives in a selective manner. Notably, depending upon the support material we could tune the selectivity of the corresponding product which will be presented during the conference.



References

1. W. Dong, and A. Didier, Chem. Rev., 2015, 13, 6621.

2. N. Garg, S. Paira and B. Sundararaju., ChemCatChem, 2020, 12, 3472.



10-13 December 2023

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To pursue research in the field of catalysis (Enzyme, Supramolecular, Homogeneous, Asymmetric, Photo, Organocatalysis) and Organometallic chemistry.

Dec 2018 – Present	<i>Assistant Professor,</i> Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology,Vellore, Tamilnadu, India.
Sep 2016 – Nov 2018	Postdoctoral Fellow with Prof. Dr. Joost N.H.Reek University of Amsterdam, Amsterdam, Netherlands
Sep 2015 – Aug 2016	Postdoctoral Fellow with Prof. Dr. Bert Maes Department of Chemistry, University of Antwerp, Antwerp, Belgium.
March 2014 – Aug 2015	Postdoctoral Fellow with Prof. Dr. Matthias Beller Leibniz-Institute for Catalysis, Rostock, Germany
Oct 2010 – Nov 2013	 Doctor of Philosophy with Prof.Dr. Henri Doucet UMR 6226-CNRS-Université de Rennes1, Rennes, France. Dissertation: Pd catalyzed C-H bond activation for simpler access to ArSO₂R derivatives
Sep 2009 – July 2010	Diplôme in Master Sciences (Chemistry) Université de Rennes1, Rennes, France. Specialized in Catalysis, Molecular and Green Chemistry. http://www.immc.univ-rennes1.fr/
June 2007 – June 2009	<i>Master of Science (Chemistry)</i> St. Joseph's College (Bharathidhasan University) Tiruchirapalli, India



FL-4

10-13 December 2023

Direct Decarboxylative C-N and C-O Bond Formation Reactions in Water Microdroplets

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Water microdroplets exhibit unusual reaction properties that are not observed in bulk water or other organic solvents.¹⁻³ Due to the advantages of hydrogen peroxide formation at the water-gas interface under the strong electric field, we and others utilized the hydroxyl radical to carry out various organic reactions.⁴⁻⁵ Nitrogen and oxygen containing organic compounds play a major role in synthesis of biologically active targets, natural products synthesis and pharmaceuticals. Several methods were available for the synthesis of nitrogen and oxygen, containing organic molecules via C-N or C-O bond formation. The existing methods requires rather harsh reaction conditions, such as use of a metal catalyst, long reaction times, irradiation at different wavelengths, and high temperatures. More economical and green methods to rapidly form C-N or C-O bonds at room temperature are still under investigation. In this talk, I will briefly discuss the direct C-N and C-O bond formation reaction from benzoic acid via decarboxylation in water microdroplets. The C-N and C-O bond formation products were obtained in one step at room temperature without metal catalyst in water.⁶⁻⁷



References

1. E. Gnanamani, X. Yan and R. N. Zare, Angew. Chem. Int. Ed. 2020, 59, 3069.

2. P. Basuri, L. E. Gonzalez, N. M. Morato, T. Pradeep and R. G. Cooks, *Chem. Sci.* 2020, 11, 12686.

3. A. Kumar, S. Mondal, Sandeep, P. Venugopalan, A. Kumar, S. Banerjee, *J. Am. Chem. Soc.* 2022, **144**, 3347.

4. L. Xue, B. Zheng, J. Sun, ACS Sustain. Chem. Eng. 2023, DOI: 10.1021/ acssus chemeng.3c03313.

5. Y. Meng, E. Gnanamani and R. N. Zare, J. Am. Chem. Soc. 2022, 144, 19709.

6. Y. Meng, E. Gnanamani and R. N. Zare, J. Am. Chem. Soc. 2023, 145, 32.

7. Y. Meng, R. N. Zare, E. Gnanamani, J. Am. Chem. Soc. 2023, Just accepted.



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Dr. E. Gnanamani is currently an assistant professor of Organic Chemistry at IIT-Roorkee. He obtained his Ph.D from Pondicherry University with Prof. C. R. Ramanathan in April 2013. In June 2013, he began a postdoctoral appointment at the ICCAS, where he researched asymmetric organocatalysis with Profs. Luo Sanzhong and Jin-Pei Cheng. In November 2014, he was awarded a Fulbright Fellowship to pursue further postdoctoral studies at Stanford University. At Stanford, he worked in Prof. B. M. Trost's group from January 2015 to March 2020 on a variety of different transition metal-catalyzed reactions. While at Stanford, Dr. E. Gnanamani also worked with Prof. R. N. Zare to develop methods of accelerating organic reactions in microdroplets. Dr. E. Gnanamani, a recipient of developing country international award and Fulbright award. Also, Dr. E. Gnanamani serving as associate editor of Current Indian Science: Organic Synthesis Journal. He has published research papers in high impact journals such as *JACS*, *Nat. Cat., Angew. Chem. Int. Ed., PNAS* etc.



IL-17

10-13 December 2023

En-Lightening C-H functionalization

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The scientific community has long sought to emulate nature's mechanisms, particularly in understanding how enzymes achieve chemical transformations with precision. Through extensive research, we have gained a thorough understanding of how enzymes catalyze the functionalization of inert C-H bonds in a regio- and stereoselective manner, utilizing metal-active sites. Taking inspiration from these natural processes, we have successfully developed catalytic methods for the functionalization of carbon-hydrogen (C-H) bonds. The Fujiwara–Moritani reaction is one of such reaction which made significant impact on the development of modern C-H activation methodologies. Despite the traditional approach's widespread applicability in various fields, issues related to reactivity and regioselectivity have limited its effectiveness. To revive this remarkable reaction, it is necessary to establish a mechanistic framework that allows simultaneous control over both reactivity and regioselectivity. The conventional high-temperature conditions required for olefination often lead to undesired multiple functionalizations at different sites.

In our work, we have successfully established a photoredox catalytic system by merging a palladium catalyst with an organo-photocatalyst (PC). This innovative system enables selective oxidative olefination of diverse arenes and heteroarenes in a highly regioselective manner. The utilization of visible light plays a crucial role in driving these "regioresolved" Fujiwara–Moritani reactions, eliminating the need for silver salts and high thermal energy. Our catalytic system also exhibits compatibility with both proximal and distal olefination, facilitated by the appropriate directing groups (DGs). This versatility allows us to engage the entire spectrum of $C(sp^2)$ –H olefination. The broad scope of this protocol allows for the synthesis of diverse compounds, including natural products, chiral molecules, and drugs. The established mechanistic insights further enhance our understanding of this reaction, enabling future advancements in this field. Importantly, this method offer significant advantages over traditional synthetic approaches, both in terms of economic feasibility and environmental impact.



References: 1. J. Am. Chem. Soc. **2022**, 144, 4; Science, **2021**, 372, 701; 2. Nat. Commun. **2021**, 12, 1393; 3. Angew. Chem. Int. Ed. **2021**, 60, 14030; 4. J. Am. Chem. Soc., **2020**, 142, 12453; 5. J. Am. Chem. Soc., **2020**, 142, 3762.



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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 an Associate Editor of *Journal of Organic Chemistry*.



10-13 December 2023

IL-18

An efficient catalyst for cross-coupling reaction: the cobalt

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Transition-metal-catalyzed cross-couplings are essential methods to build C-C bonds for the synthesis of pharmaceuticals and natural products, since the pioneering work of Heck, Negishi, and Suzuki. Among the widely used group 8–10 metal catalyst, economical cobalt salts advantageously replace expensive and toxic catalysts for cross-coupling reactions. In this lecture, we will present some cobalt-catalyzed reductive cross-couplings using cheap and abundant electrophiles such as C-O/C-CN/C-S electrophiles as versatile and sustainable synthetic tool instead of organic halides for selective C-C bond formation.¹

In the first part, we will show the Co-catalyzed cross-coupling of aryl chlorides with benzonitriles. In the second part, we will present various crosselectrophilic coupling involving benzylic compounds and alkyl or aryl compounds.



References

- C. Dorval, M. Tricoire, J.-M. Begouin, V. Gandon, C. Gosmini, ACS Catal., 2020, 10, 12819

- C. Dorval, O. Stetsiuk, S. Gaillard, E. Dubois, C. Gosmini, G. Danoun, Org. Lett., 2022

- B. R. Prasad Reddy, S. Chowdhury, A. Auffrant, C. Gosmini, *Adv.* Synth. Catal., 2018, 360, 3026.

- H. Fillon, C. Gosmini, J. Périchon, J. Am. Chem. Soc., 2003, 125, 3867

- M. Gao, C. Gosmini, Adv. Synth. Catal., 2023 accepted.

- X. Qian, A. Auffrant, A. Felouat, C. Gosmini, Angew. Chem. Int. Ed. 2011, 123, 10586.



10-13 December 2023

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Corinne Gosmini was born near Paris in France. She obtained her PhD in chemistry at Université Pierre et Marie Curie (Paris, France) under the guidance of Professor Jean F. Normant and Dr Raymond Sauvêtre. In 1993, she was appointed by the CNRS as « Chargée de Recherches » in the laboratory of Professor Jacques Périchon. She is currently CNRS Director of Research at the « Laboratoire de Chimie Moleculaire » and was associate Professor at the Ecole Polytechnique (2012-2023 at Palaiseau - France). From 2013 to 2020, she was the head of the « Laboratoire de Chimie Moleculaire ». During 2020-21, she was in charge of a mission for the CNRS chemistry Institut. Since 2022, she is an expert on several laboratory evaluation committees. Her early interests were devoted toward the development of new electrochemical reactions catalyzed by nickel and mainly cobalt complexes. Since 2003, her main research activities focused on the development of new chemical Cocatalyzed cross-coupling reactions and preparations of organometallic compounds (especially organozinc species) under versatile conditions in order to form C-C and C-heteroatom bonds using this same cobalt catalysis. She was the first to develop electrophilic cross-couplings with a first row metal from C-halides bonds and now she is studying Co-catalyzed cross-coupling reactions from non-activated bonds such as C-O, C-N and C-C bonds. In 2022, she was a distinguished member of the Société Chimique de France. She is the author of more than 100 publications and 11 patents.



IL-19

10-13 December 2023

Aromatic metamorphosis

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Aromatic rings hold a central position in organic chemistry and govern the fundamental nature of numerous aromatic compounds. Aromatic rings are stable due to their aromatic resonance energy and thus usually considered as Compared with exocyclic modifications of aromatic being unbreakable. compounds, little is known about endocyclic modifications such as substitutions of endocyclic atoms and atom insertions into the rings through partial disassembly of the cyclic skeletons and subsequent ring reconstruction. For the last decade, we have been interested in developing a series of new synthetic methods to achieve endocyclic modifications of heteroarenes as a game-changing strategy in organic synthesis. I will talk about our endeavors to metamorphosis',¹⁻³ establish 'aromatic focusing on the catalytic transformations of heteroaromatic skeletons.⁴⁻⁶



References

1. H. Yorimitsu, D. Vasu, M. Bhanuchandra, K. Murakami and A. Osuka, *Synlett* 2016, 27, 1765.

- 2. K. Nogi and H. Yorimitsu, Chem. Commun. 2017, 53, 4055.
- 3. H. Saito and H. Yorimitsu, Chem. Lett. 2019, 48, 1019.
- 4. D. Vasu, H. Yorimitsu and A. Osuka, Angew. Chem. Int. Ed. 2015, 54, 7162.
- 5. H. Saito, S. Otsuka, K. Nogi and H. Yorimitsu, J. Am. Chem. Soc. 2016, 138, 15315.
- 6. S. Tsuchiya, H. Saito, K. Nogi and H. Yorimitsu, Org. Lett. 2017, 19, 5557.



10-13 December 2023

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Education

2002-03 Postdoctoral Fellow, The University of Tokyo (Prof. Eiichi Nakamura)2002 PhD, Kyoto University (Prof. Koichiro Oshima)

1997 BS, Kyoto University

Academic Careers

2015- Professor, Department of Chemistry, Kyoto University

2009-15 Associate Professor, Department of Chemistry, Kyoto University

2008-09 Associate Professor, Department of Material Chemistry, Kyoto University

2003-08 Assistant Professor, Department of Material Chemistry, Kyoto University

Recent Representative Professional Service

Co-Chair, 22nd International Symposium on Organometallic Chemistry Directed Toward Organic Synthesis (OMCOS-22, 2025); Chair, International Kyoto Next-Generation Organic Chemistry Symposium (KNOCS, 2023-); Organizer, Tateshina Conference on Organic Chemistry (2023-); Associate Editor for SYNTHESIS (2019-).

Recent Selected Honors

2023 Swiss Chemical Society Lectureship Award

- 2022 Visiting Professor, National Chung Hsing University, Taiwan
- 2020 Japan Academy Medal

2020 JSPS Prize

- 2018 Honorary Chair Professor, National Taipei University of Technology
- 2018 Negishi Award (from Japan Science and Technology Agency)
- 2016 Mukaiyama Award (from the Society of Synthetic Organic Chemistry, Japan)
- 2011 The Young Scientists' Prize (from the MEXT Minister)

Recent Selected Publications

(i) "Stereo- and regioselective boryllithiation and -sodiation of arylacetylenes using flow microreactors" *Nat. Synth.* 2024, **3**, *in press.* (ii) "Synthesis of *trans*-1,2-dimetalloalkenes through reductive *anti*-dimagnesiation and dialumination of alkynes" *Nat. Synth.* 2023, **2**, 162. (iii) "Utilization of Silanols in Transition Metal-Catalyzed Organic Synthesis" *ACS Catal.* 2023, **13**, 7472. (iv) "Sulfur(IV) in Transition-Metal-Free Cross-Couplings for Biaryl Synthesis" G. J. P. Perry and H. Yorimitsu, *ACS Sustainable Chem. Eng.* 2022, **10**, 2569. (v) "Catalytic Transformations of Sulfonium Salts via C–S Bond Activation" *Chem. Rec.* 2021, **21**, 3356. (vi) "Carbon–Carbon Bond Cleavage at Allylic Positions: Retro-allylation and Deallylation" *Chem. Rev.* 2021, **121**, 345.





IL-20

10-13 December 2023

Transition Metal-Catalyzed Enantioselective C-H Functionalization

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In the past decade, metal-catalyzed enantioselective C-H activation has emerged as a powerful approach to access chiral molecules. Previous methods mainly rely on the use of noble metal catalysts.¹ Considering the earth-abundance, inexpensiveness, and, most importantly, the unique and versatile reactivity of cobalt catalysts, we have engaged in the development of cobalt-catalyzed enantioselective C-H functionalization reactions recently. We have developed three novel types of cobalt catalysis, namely, achiral CpCo(III)/chiral carbonyl acid (CCA),² Co(II)/chiral spiro phosphoric acid (SPA) cooperative catalysis,³ and Co(II)/salicyloxazoline (Salox),⁴ which enable the highly enantioselective synthesis of chiral molecules bearing planar chirality, axial chirality, C- and P-stereogenic centers. We also realized the first electrooxidative cobalt-catalyzed enantioselective C-H activation reaction.⁵



References

- a) Zhang, Q.; Shi, B.-F. Acc. Chem. Res. 2021, 54, 2750; b) Zhan, B.-B.; Jin, L.; Shi, B.-F. Trends in Chem. 2022, 4, 220. 2.
- Liu, Y.-H.; Xie, P.-P.; Liu, L.; Fan, J.; Zhang, Z.-Z.; Hong, X.; Shi, B.-F. J. Am. Chem. Soc. 2021, 143, 19112.
- 3. Yuan, W.-K.; Shi, B.-F. Angew. Chem. Int. Ed. 2021, 60, 23187.
- 4. Yao, Q.-J.; Chen, J.-H.; Huang, F.-R.; Shi, B.-F. Angew. Chem. Int. Ed. 2022, 61, e202202892.
- 5. Yao, Q.-J.; Huang, F.-R.; Chen, J.-H.; Zhong, M.; Shi, B.-F. *Angew. Chem. Int. Ed.* 2023, 62, e202218533.



10-13 December 2023

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Bing-Feng Shi was born in Shandong, China. He received his B.S. degree from Nankai University in 2001 and a Ph.D. degree from the Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences under the guidance of Professor Biao Yu in 2006. Following time as a postdoctoral fellow at the University of California, San Diego (2006–2007), he moved to The Scripps Research Institute working with Professor Jin-Quan Yu as a research associate. In 2010, he joined the Department of Chemistry at Zhejiang University as a professor. He is now Qiushi Distinguished Professor and Executive Dean of the department and also serves as an associate editor of The Journal of Organic Chemistry. His research focus is transition metal-catalyzed C–H functionalization and the application in the synthesis of biologically important small molecules.



IL-21

10-13 December 2023

Catalyst development for sustainable oxidation reactions

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Catalysts that selectively oxidize C-H bonds and mimic natural Fe-containing enzymes have the power to re-orient organic synthesis. Although iron complexes are known to activate H₂O₂ to perform selective oxidation of unactivated C-H bonds, all of them only operate in organic solvents. It is extremely challenging to design synthetic iron complexes that perform selective C-H oxidation in nature's solvent "water" (mimicking the metalloenzyme cytochrome P450). In this talk, I will discuss designing iron complexes that even in the absence of a protein scaffold can activate H2O2 and perform very selective, fast, and scalable C-H oxidation in complex organic molecules including natural products in 100% water. This iron complex, a modified "picket-fence" Fe-bTAML complex, can oxidize C-H and C=C bonds in several organic substrates with low catalyst loadings (1-4 mol%) and a small excess of H_2O_2 (2-3 equiv) in water. Subsequently, I will discuss strategies for the exclusion of solvent from these C-H oxidation reactions under mechanochemical conditions. Applications of such solvent-free reactions in the upcycling of commercial hydrocarbon polymers will be discussed.

References

Sandipan Jana et. al. Chemical Science, 2023, DOI: 10.1039/D3SC03495J.

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Sayam Sen Gupta did his undergraduate degree in Chemistry from University of Kolkata followed by his masters at IIT-Kanpur. He then moved to United States where he finished his doctoral degree from Carnegie Mellon University at Pittsburgh. After two post-doctoral stints in US and Germany (Alexander von Humboldt Fellow), he joined NCL as a scientist in December 2006 where he was a Senior Scientist in the Chemical Engineering Division. He moved to IISER-Kolkata in 2016 as an Associate Professor and is currently Professor in the Department of Chemical Sciences. He is an inorganic chemist by training and works in the broad area of sustainability, particularly in bio-inspired catalysis and materials. He also teaches Sustainability and Chemistry at IISER Kolkata, a course which he co-developed.



IL-22

10-13 December 2023

Polydopamine-coated polyurethane foams as a versatile catalytic support: illustration with a Pd-functionalized foam and its application as a highly reusable catalyst in a "dip-and-play" mode for selective alkyne semi-hydrogenation and aerobic Suzuki coupling

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Structured Catalytic Supports (SCS) are widely used in continuous processes. Among the variety of SCS, open cell foams are prime candidates. In this context, our group has recently proposed the use of flexible, mechanically resistant and inexpensive polyurethane foams (PUF) as an alternative to expensive and fragile metallic and ceramic foams. PUF can indeed be readily coated with a thin layer of polydopamine (PDA) - inspired by the mussels' adhesion principle [1] - which then allows the robust grafting of both inorganic particles and molecular compounds [2].

The selective hydrogenation of alkynes to alkenes covers an important area of industrial production. Supported catalysts containing Pd nanoparticles are among the best candidates in terms of activity, but they often suffer from moderate selectivity. An effective approach to improve it relies on the "active site isolation" strategy, dealing with the development of single atom-based catalysts. This strategy however requires complex and costly synthetic solutions that compromise the process sustainability and its large-scale implementation.

In this context, we will present a straightforward catalyst preparation based on the simple immersion of the structured support, PDA@PUF, in a hydroalcoholic solution of a Pd(II) salt. The as-prepared catalyst, Pd@PDA@PUF, acts as an efficient and highly reusable heterogeneous catalyst, without priorreduction processes, for the selective semi-hydrogenation of alkynes, as well as for the Suzuki coupling of aryl bromides under aerobic conditions.

Thorough characterizations suggest an initial coordination of the Pd(II) ions by the catechol moieties of the PDA layer, resulting in a single atom-type dispersion of the active phase that would be at the origin of Pd@PDA@PUF's high alkene selectivity in alkyne hydrogenation catalysis, and a progressive reduction of Pd(0) Pd(II) into under catalytic conditions [3].



References

[1] H. Lee, S. M. Dellatore, W. M. Miller, P. M. Messersmith, *Science* 2007, **318**, 426.
[2] (a) E. Pardieu, N. T. T. Chau, T. Dintzer, T. Romero, D. Favier, T. Roland, D. Edouard, L. Jierry, V. Ritleng, *Chem. Commun.* 2016, **52**, 4691. (b) A. Ait Khouya, M. L. Martinez Mendez, P. Bertani, D. Favier, T. Roland, V. Guidal, V. Bellière-Baca, D. Edouard, L. Jierry, V. Ritleng *Chem. Commun.* 2019, **55**, 11960.

[3] H. Peng, V. Papaefthimiou, T. Romero, C. Pham-Huu V. Ritleng, *Green Chem.* 2023, **4**, 2265.



10-13 December 2023

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Vincent Ritleng was educated at the University Louis Pasteur (Strasbourg, France), where he studied ruthenium-mediated C-H bond activation and C-C bond formation and received his PhD in 2001 under the supervision of Dr. Michel Pfeffer. He then joined the Massachusetts Institute of Technology (USA), where he worked on dinitrogen reduction to ammonia with triamidoamine molybdenum complexes as a postdoc of Pr. Richard R. Schrock (2001-2003). A second postdoc with Pr. Ben L. Feringa and Pr. Johannes G. de Vries at the University of Groningen (Netherlands) allowed him to work on chiral alcohol racemization with the aid of ruthenacycles. He was then appointed Maître de Conférences (Associate Professor) in 2004 at the European School of Chemistry, Polymers and Materials (ECPM) of the University of Strasbourg. In 2012, he was made Fellow of the University of Strasbourg Institute for Advanced Study, in 2014, he was nominated Junior Member of the "Institut Universitaire de France", and in 2018, he was promoted Full Professor. He is the coauthor of 55 papers (h = 26, > 4760 citations) and co-owner of 3 patents with PCT. His current research interests involve the development of (i) nickel complexes bearing NHC ligands for hydrofunctionalization, cross-coupling, and C-H bond functionalization reactions, and (ii) of catalytic supports, either structured at the macroscopic scale or organized at the molecular scale.



SL-5

10-13 December 2023

High valent Nickel Species: Synthesis and Characterization

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Nature's extremely vital metalloenzymes, *i.e.*, Cytochrome P450s and Galactose Oxidases exploit non-innocent ligands to form reactive high valent intermediates for oxidation reactions.¹ This strategy works well for the late 3d metals where accessing high valent states is rather challenging.² In this regard, Ni^{II}(salen) complexes have been one of the most promising avenues for those aiming to generate high valent Ni species.^{3, 4} This talk is based on one such inquisitiveness where a Ni^{II}(salen) (Figure 1) was treated with mCPBA to form a novel Ni(III) bisphenoxyl diradical species, formally analogous to a high valent Ni(V) species. Electrochemical and spectroscopic analyses using UV-Vis and EPR further revealed oxidation events on the ligand as well as on the metal centre to yield a Ni(III) bisphenoxyl diradical species, Ni^{III}(L^{••}).⁵ Further, we studied the conditions (*i.e.*, addition of exogenous ligands like pyridine and guinoline) that alter this equilibrium and decides where an effective unpaired electron would localize in Ni(III) bisphenoxyl diradical species. However, the use of mCPBA limits the disclosure of the processes involved in the production of a formal Ni(V)species. Therefore, by varying the potential and concentration of an electron transfer oxidant, CAN with acid along with the temperature, we also observed that the formation of intermediate species such as Ni(III) and a formal Ni(IV) prior to the generation of a *formal* Ni(V) species in CH₃CN. This study benefits the pioneers in understanding the mechanisms of the crucial systems, where now a presence of high valent species like a formal Ni(V) could also be plausible. The intermediates discussed here have also been explored as a potential candidate for vital OAT, HAT or ET reactivities making them one of the likely intermediate in Ni-salen catalyzed oxidation reactions.



Figure 1. Scheme depicting the strategies to form various oxidizing species with 1 to date.

References

(1) Itoh, S.; Taki, M.; Fukuzumi, S.; *Coord. Chem. Rev.* 2000, *198*, 3–20. (2) Shimazaki, Y.; Tani, F.; Fukui, K.; Naruta, Y.; Yamauchi, O.; *J. Am. Chem. Soc.* 2003, *125*, 10512–10513.
(3) Storr, T.; Wasinger, E. C.; Pratt, R. C.; Stack, T. D. P.; *Angew. Chemie. Int. Ed.* 2007, *46*, 5198–5201. (4) Dunn, T. J.; Webb, M. I.; Hazin, K.; Verma, P.; Wasinger, E. C.; Shimazaki, Y.; Storr, T.; *Dalt. Trans.* 2013, *42*, 3950–3956.

(5) Awasthi, A.; Leach, I. F.; Engbers, S.; Kumar, R.; Eerlapally, R.; Gupta, S.; Klein, J. E. M. N.; Draksharapu, A.; *Angew. Chemie Int. Ed.* **2022**, *61*, 202211345.



10-13 December 2023

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Apparao (Appu) studied at the University of Hyderabad (India), where he completed his master thesis under the supervision of Prof. Tushar Jana. Appu then moved to University of Groningen (The Netherlands) for PhD degree (2009-13), worked in the groups of Prof. Wesley R. Browne and Prof. Bernand L. Feringa. His work mainly focused on the electro- and photochemical properties of inorganic metal complexes relevant to biological systems. He moved to University of Minnesota (United States) to work with Prof. Lawrence Que, Jr. on bio-mimetic iron complexes. Currently, he is working at IIT Kanpur as an assistant professor.

Many of the challenging chemical transformations indispensable for chemical industries can often be carried out by nature under ambient conditions with remarkable reactivity and selectivity. Developing artificial metalloenzymes to catalyze abiological reactions has been a major endeavor for many years, but most of the times the observed rate of the synthetic mimics is lower than those of metalloenzymes, making them unsuitable for practical applications. A critical step to advance the field is to fundamentally understand what it takes to not only support the high valent metal species but also modulate the reactivities of those artificial synthetic mimics. Appu's biomimetic group strives to imitate high valent metal species found in the biological systems through spectroscopic characterization, to get a mechanistic understanding of the crucial processes.



SL-6

10-13 December 2023

Bioinspired Aromatic Hydroxylation: Role of Redox-Active Metals

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Phenol is the starting material for synthesizing several industrially valuable chemical products. It is manufactured only by a three-step cumene process using benzene and dioxygen, which shows a yield of \sim 5%. Therefore, developing a single-step methodology is crucial for synthesizing phenol from benzene. Its high C-H bond energy (460 kJ mol⁻¹) and the lack of kinetic control of phenol oxidation over benzene hamper the higher yields. However, naturally occurring oxygenases are known to activate these C-H bonds at ambient conditions using dioxygen. We have reported the Ni(II) complexes of ligands [Ni^{II}(N₄)(CH₃CN)₂]²⁺ as bioinspired catalysts for benzene N₄ hydroxylation. It showed a maximum of 41% phenol formation using H_2O_2 as an oxidant by the involvement of short-lived key intermediate species $[(N_4Ni^{III})_2(\mu-O)_2]^{2+}$. However, the Co(II) complexes of the identical ligands favored Co(III)-hydroperoxo for the benzene to phenol conversion, which showed only a 29% yield. Interestingly, the Cu(II) complexes of the same ligand series afforded 37% of phenol from benzene via Cu(II)-OOH intermediate. The Fe(II) analogs showed a 21% yield of phenol occurred via [(L)Fe^{III}-OOH] species or its high-valent species. The ligand architecture and redox potentials varied the catalytic efficiency of complexes. Our methodology is the new biomimetic catalytic process for phenol formation from benzene via the greener pathway at a single step.



Scheme 1. The metalloenzymes are known to perform hydroxylation (left) and benzene hydroxylation reactions by our bioinspired catalysts (right).

References

1. R. Mayilmurugan and coworkers, (a) *Catal. Sci.Technol.*, **2019**, *9*, 5991-6001. (b) *Catal. Sci. Technol.* **2020**, *10*, 2540-2548. (c) *Inorg. Chem.*, **2020**, 59, 5918-5928. (d) *Dalton Trans.* **2020**, *49*, 13829 -13839. (d) *J. Catalysis* **2019**, *372*, 352.



10-13 December 2023

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RESEARCH INTEREST: Bioinorganic Chemistry and Bioinspired Catalysis: Small Molecule Activation (O₂ and CO₂) by Bioinspired Approach- Inorganic Chemical Biology: Smart PARACEST and T1- MRI-Contrast Agents - Optical Imaging Probes.

ACADEMIC BACKGROUND

- Fulbright Scholar, University at Buffalo, State University of New York, USA (Mentor: Prof. Janet R Morrow, Assoc. Editor, Inorganic Chemistry)
- 2009-2010 : Post-Doctoral Research Associate, Karl-Franzens-Universität Graz, Austria (Mentor: Prof. Nadia C. Mösch-Zanetti)
- 2003-2008 : Ph.D. School of Chemistry, Bharathidasan University
- 2000–2002 : M.Sc. Madurai Kamaraj University
- 1997-2000 : B.Sc. Madurai Kamaraj University

PROFESSIONAL EXPERIENCE

- Jan. 2022–Present: Assistant Professor, Department of Chemistry, IIT-Bhilai
- 2011–2021 : Assistant Professor, School of Chemistry, Madurai Kamaraj University, India.

AWARDS AND RECOGNITIONS

- CRSI Bronze Medal (2020), Chemical Research Society of India (CRSI)
- CRSI Council Member (2020-23)
- Fulbright Outreach Fund (2015)
- Fulbright Scholar Award (2014), Fulbright Commission in India (USIEF)
- DFG-INSA Fellowship to Germany (2014)
- DST Young Scientist Project Award (2012)
- Foreign Travel Grant by DST and CSIR to Germany (2005)
- CSIR-NET (2003) and CSIR-Senior Research Fellowship(2005), India
- Gold medal for securing the first rank in M.Sc (2002)
- Tamil Nadu State Government Post Graduate Student Project Award (2002).

VISITING PROFESSORSHIP

- Royal Institute of Sweden, Stockholm (December 2013)
- Heidelberg University, Germany (May –July 2014)
- Karl-Franzens-Universität Graz, Austria (Sep.-December 2013)
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RESEARCH PROJECTS AND STUDENT GUIDED

- Completed Projects: 7 (DST, SERB, BRNS, DBT and UGC)
- Ongoing: 3 (SERB, IIT Bhilai, RIG)
- PhD student Guided: 7 Ongoing -4; Master Student Guided: 24.

PUBLICATIONS: Total published: 51; h-index: 21; i-10 index: 34.



IL-23

10-13 December 2023

From Reduction to Alkylation: A Journey with Iron Complexes

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Economic constraints and environmental concerns in chemistry have led to increased demand for the replacement of noble metals used in chemical processes by Earth-abundant ones. Iron-catalyzed reduction has received intensive attention and some iron complexes have shown activities and selectivities that are competitive with those of noble metals.^[1] However, replacing noble metals by cheap, abundant, and biocompatible iron complexes to perform reduction is not the sole criterion to render such complexes attractive for industrial applications, the catalytic activities and the price of the ligand must also be taken into account.^[2] In our ongoing research on ironcatalyzed reduction,^[3] some new cyclopentadienone iron tricarbonyl complexes have been designed based on a "transition metal frustrated Lewis approach.^[4] Their application in chemoselective pair" thermal or photoactivated alkylation, as well as a detailed mechanistic study will be presented.^[5]

References

1. a) D. Wei, C. Darcel, *Chem. Rev.* **2019**, *119*, 2550-2610. b) L. Alig, M. Fritz, S. Schneider, *Chem. Rev.* **2019**, *119*, 2681-2751.

2. P. Dupau, M.-L. Tran Do, S. Gaillard, J.-L. Renaud, *Angew. Chem. Int. Ed.* **2014**, *53*, 13004-13006.

3. A. Pagnoux-Ozherelyeva, N. Pannetier, M. D. Mbaye, S. Gaillard, J.-L. Renaud, *Angew. Chem. Int. Ed.* **2012**, *51*, 4976-4980. b) A. Lator, S. Gaillard, A. Poater, J.-L. Renaud, *Chem. Eur. J.* **2018**, *24*, 5770-5774

4. a) T.-T. Thai, D. S. Mérel, A. Poater, S. Gaillard, J.-L. Renaud, *Chem. Eur. J.* **2015**, *21*, 7066-7070. b) A. Lator, Q. Gaignard Gaillard, D. S. Mérel, J.-F. Lohier, S. Gaillard, A. Poater, J.-L. Renaud, *J. Org. Chem.* **2019** *84*, 6813-6829.

5. a) M.S. Abdallah, N. Joly, S. Gaillard, A. Poater, J.-L. Renaud, *Org. Lett.* 2022, *24*, 5584-5589. b) L. Bettoni, S. Gaillard, J.-L. Renaud, *Chem. Commun.* 2020, *56*, 12909-12912. c) L. Bettoni, S. Gaillard, J.-L. Renaud, *Org. Lett.* 2020, *22*, 2064-2069. d) L. Bettoni, C. Seck, M. D. Mbaye, S. Gaillard, J.-L. Renaud, *Org. Lett.* 2019, *21*, 3057-3061. e) A. Lator, S. Gaillard, A. Poater, J.-L. Renaud, *Org. Lett.* 2018, *20*, 5985-5990.



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Prof. Jean-Luc Renaud obtained his Ph.D. degree in 1998 under the supervision of Dr. Aubert and Prof. Malacria. He was a Lavoisier Postdoctoral fellow in 1999 with Prof. Lautens at the University of Toronto then moved to the University of Louvain-La-Neuve in the team of Prof. Riant. In 2000, he was appointed as Maître de Conférences at the University of Rennes and accepted a full Professor position at University of Caen Normandy in 2008. He is being invited researcher at the "Institut Parisien de Chimie Moléculaire (IPCM), Sorbonne University, since October 2023. The research interests focus on organometallic catalysis, organocatalysis, photoredox catalysis and their application towards the synthesis of biologically interesting molecules and processes relevant to fine chemical synthesis.

Award: 2022 Dalton Division Horizon Prize (<u>https://www.rsc.org/prizes-funding/prizes/2022-winners/cu-lighting/#undefined</u>)



IL-24

10-13 December 2023

Iron-catalyzed Hydrosilylation, Alkoxylation and Tandem Hydrosilylative-Alkoxylation

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Late transition metals such as rhodium, iridium, etc. are the preferred metals for various transformations like hydroformylation, hydrosilylation, carboxylation, alkoxylation, etc.¹ However, later transition metals are precious, costly, and rare. Therefore, recent literature has witnessed the usage of early transition metals, such as iron, in homogeneously catalyzed transformations.² My lecture will take stock of challenges in iron-catalyzed transformations, briefly discuss the current solution, and reiterate the enormous potential of iron in metal-catalyzed transformations. I shall present 3-4 case studies from my research group and demonstrate the untapped potential of iron as presented in Figure 1.³



Figure 1: Iron-catalyzed transformations.

References

R. Franke, D. Selent and A. Boerner, *Chem. Rev.* 2012, **112**, 5675-5732.
 S. Pandey, K. Vipin Raj, D. R. Shinde, K. Vanka, V. Kashyap, S. Kurungot, C. P. Vinod and S. H. Chikkali, *J. Am. Chem. Soc.* 2018, **140**, 4430-4439
 A. Sen, T. Tewari, R. Kumar, R. G. Gonnade and S. H. Chikkali, *Chem. Eur. J.* 2023, DOI:10.1002/chem.202301375.



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Samir Chikkali earned his Ph.D. under the supervision of Prof. Dietrich Gudat from the University of Stuttgart, Germany. Subsequently, he did postdoctoral research with Prof. Joost Reek at the University of Amsterdam, the Netherlands, and Prof. Stefan Mecking at the University of Konstanz, Germany. In 2012 he returned to India and joined CSIR-National Chemical Laboratory (CSIR-NCL), Pune, to start his independent research career. He has guided 8 Ph.D. students, 6 post-docs, and 15 project assistants. Currently, he leads a team of 18 highly motivated researchers in organometallics, polyolefins, and renewable/degradable polymers. His scientific interests are- organometallics, olefin polymerization, renewables to polymers, asymmetric hydrogenation/hydroformylation, and depolymerization. His honours and awards include a summer fellowship from the Indian Academy of Science, DPI (Dutch Polymer Institute) postdoctoral fellowship, AvH (Alexander von Humboldt) postdoctoral fellowship, the Ramanujan (DST) Fellowship, Best Scientist Award by North Maharashtra University, Scientist of the Year Award 2016-2017 & 2022-2023 by NCL-RF, Young Associate of Maharashtra Academy of Sciences 2017, Professor Kaushal Kishore Memorial Award 2020 by Society of Polymer Science, India (SPSI), and 10th National Award 2020, by Ministry of Chemicals and Fertilizers, Government of India.

His research in organometallic catalysis has been rightly recognized by peers with top-quality publications and has been equally applauded by the industry with sponsored/consultancy projects. He has published over 68 papers in international journals of high repute, he is an inventor on 11 patents and has edited a book on metal-catalyzed polymerization (<u>https://www.taylorfrancis.com/books/metal-catalyzed-polymerization-samir-chikkali/e/10.1201/9781315153919</u>).

He has served as guest editor of "Journal of Chemical Sciences" in the past (July 2018 issue). He has been appointed as an "Associate Editor" of "Bulletin of Materials Science" (since 1st Jan. 2023 for a period of 3 years.



IL-25

10-13 December 2023

Catalytic Cascade Transformations for Polyheterocycles Synthesis

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Catalytic cascade transformations are powerful synthetic methods used in organic chemistry to efficiently construct complex molecules from simple starting materials in a single reaction vessel. These transformations involve multiple catalytic steps occurring sequentially in a domino fashion. In this presentation, we will be providing some of the methods designed around bringing a couple of sequential transformations in one pot to construct the nitrogen and/or oxygen containing polyheterocycles having the potential applications in medicinal chemistry and materials science. Some of these transformations are funded on generating reactive intermediates such as carbenes and/or nitrenes and inter-/intramolecular trapping and subsequent rearrangements.



References

- 1. Patel, P.; Ramana, C. V. Org. Biomol. Chem. 2011, 9, 7327–7334.
- 2. Dhote, P. S.; Ramana, C. V. Org. Lett. 2019, 16, 6221–6224.
- 3. Dhote, P. S.; Ramana, C. V. Org. Lett. 2021, 23, 2632–2637.
- 4. Dhote, P. S.; Pund, K.; Ramana, C. V. J. Org. Chem. 2021, 86, 10874-10882.
- 5. S. V. Halnor; P. S. Dhote C. V. Ramana Org. Biomol. Chem. 2023, 21, 2127-2137.



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Dr. Ramana obtained his MSc. from Andhra University,

Waltair (1991) and PhD from University of Hyderabad under the supervision of Professor M. Nagarajan (Synthetic Carbohydrate Chemistry). From 1998 to 2001 he was associated with Professor Andrea Vasella at ETH Zurich as a post-doctoral researcher (glycosidase inhibitors). From May 2001 onwards, he had been associated with National Chemical Laboratory (CSIR, India). At NCL, the focus of Ramana's group includes small molecules synthesis by employing transition metal complexes and developing new catalytic methods. The major focus of Dr. Ramana's group is the total synthesis of natural products and biologically important targets with a keen insight into developing new methods and extending the platform for the synthesis of pharmaceutically relevant small molecules. In general, his group is known decorating the total synthesis canvas with metal reagents and demonstrate designing of new synthetic tools involving the orchestration of sequential events in one-pot with one catalyst. In addition to this, his group also works in the areas of beta-peptides, C-saccharides synthesis, glyconanoparticles and application of C–H activation in non-infringing processes development.

He is a recipient CSIR Young Scientist award in Chemical Sciences (2003), NCL's Scientist of the Year award (2009), Professor D. K. Banerjee Memorial Lecture Award - IISc Bangalore (2011) and CRSI Bronze Medal in chemical sciences (2013) and Dr. A.V. Rama Rao Foundation Prize Lecture in Chemistry (2016) and CNR Rao National Prize in Chemical Sciences (2017). He is the fellow of Indian Academy of Sciences (2014, Bengalore). To his credit, he had 150 publications, 17 patents and 26 students have been awarded PhD. degree under his supervision.



IL-26

10-13 December 2023

Nonlinear Behaviour and the Limits of Mechanistic Understanding in Asymmetric Catalysis

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Asymmetric amplification is a phenomenon that plays a key role in the emergence of homochirality in life. In asymmetric catalysis, theoretical and experimental models have been investigated for understanding how chiral amplification is possible, in particular through non-linear effect.¹ Recently we have proposed models that have led to an understanding of more complex non-linear effects, such as hyperpositive and enantiodivergent non-linear effects, which include a coexistence of active monomeric and active dimeric species.^{2,3} A higher degree of complexity seems attainable if one considers that higher levels of aggregation could be envisaged.⁴

We show here how different ligands, issued from the same privileged chiral structure, exhibit completely different systems-level behaviours and thus also different reaction outcomes – although they differ only by small chemical modifications. Mechanistic studies showed that the metal complexes aggregate and generate additional catalytic species in distinct ways. These results were obtained through a combination of nonlinear effect studies and other related studies and simulations have confirmed the possibility of such systems-level behaviour.

Overall, these results highlight the need to be cautious with certain paradigms of asymmetric catalysis, as structures alone do not necessarily predict systems-level behaviour that could bias the outcome of the catalytic reaction.

References

- 1. Guillaneux, D.; Zhao, S.-H. ; Samuel, O. ; Rainford, D.; Kagan, H. B. *J. Am. Chem. Soc.* **1994**, *116*, 9430–9439.
- 2. Geiger, Y.; Achard, T.; Maisse-François, A.; Bellemin-Laponnaz, S. Nat. Catal. 2020, 3, 422-426.
- 3. Geiger, Y.; Achard, T.; Maisse-François, A.; Bellemin-Laponnaz, S. *Chem. Sci.* **2020**, *11*, 12453-12463.
- 4. Thierry, T.; Geiger, Y.; Bellemin-Laponnaz, S. *ChemRxiv* **2023**, doi.org/10.26434/chemrxiv-2023-qgm7t.



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S. Bellemin-Laponnaz is a CNRS research director at the Institut de Physique et Chimie des Matériaux de Strasbourg, France. He studied at the Université Joseph Fourier (Grenoble), the University of Strasbourg and the Massachusetts Institute of Technology (USA). His research interests are in the field of organometallic chemistry and coordination chemistry, with a focus on applications such as -asymmetric-catalysis, bioinorganic chemistry or materials science. He was awarded the Bronze Medal of the CNRS in 2005, the Coordination Chemistry Prize of the Société Chimique de France in 2009 and the Sandmeyer Prize of the Swiss Chemical Society in 2013. He is currently president of the Coordination Chemistry Division of the French Chemical Society and member of the scientific advisory board of the company Ineo Tech.


FL-5

10-13 December 2023

Nickel (0) Catalyzed Reductive Coupling of Aldehydes and Alkynes Over the Benchtop

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Nickel (0) complexes have been traditionally stored and used under highly controlled environments. Our research focuses on bringing sensitive nickel chemistry to the benchtop. We have demonstrated the potential of Schrauzer's Ni(COD)(Duroquinone),¹ an air-, and moisture-stable Ni⁰ complex as a catalyst for the reductive coupling of aldehydes and alkynes.² Control experiments revealed the exceptional bench stability of Ni(COD)(DQ) under ambient conditions for >200 days. The infrastructural cost associated with a glove box for storing and handling Ni(COD)₂ is avoided. A wide range of aromatic and aliphatic aldehydes/alkynes furnished the desired silvl allyl ethers in excellent yields and regioselectivities. Ynamides participate in the reductive coupling with aldehydes to give tri-substituted ene-carbamates as a regioisomer. Downstream functionalizations single like desilvlation. hydrogenation, ring-opening of epoxide, and reductive cleavage of the enecarbamate have been performed.



References

- 1. G. N. Schrauzer and H. Thyret, Naturforsch. 1962, 17, 73-76.
- 2. V. T. Tran, Z.-Q. Li, O. Apolinar, J. Derosa, M. V. Joannou, S. R. Wisniewski, M. D. Eastgate, K. M. Engle, *Angew. Chem. Int. Ed.* 2020, **59**, 7409-7413.
- 3. G. M. Mahandru, G. Liu, J. Montgomery, J. Am. Chem. Soc. 2004, 126, 3698-3699.
- 4. N. Saito, T. Katayama, Y. Sato, Org. Lett. 2008, 10, 3829-3832.



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Venkataraman Ganesh received his early education from Bishop Heber College Tiruchirapalli (2000) and joined the Integrated Ph.D. program (Chemical Sciences) at 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 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 Univ. of Bristol, UK. He started his independent research career in 2018 at the Dept. of Chemistry, Indian Institute of Technology Kharagpur, India, and holds the Ramanujan fellowship (SERB, India). His research interests include exploiting transition-metal catalysts and boron chemistry towards developing new synthetic methodologies and mechanistic studies.



FL-6

10-13 December 2023

Harnessing Non-covalent Interaction in Catalysis

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Non-covalent interactions (NCIs) like π - π stacking interactions, H-bonding, halogen bonding, anion- π interactions, XH- π interactions are ubiquitously found in both chemical and biological domains and extensively used to build new molecules and materials.¹ NCIs involving aromatic functional groups lead to molecular recognition, catalysis, stereo- and regioselectivity of the products. In a recent study we predicted the unique role of indole molecules which stabilizes the transition states during the dehydrogenation process of polyfluorinated alcohols, through non-covalent π - π and H-bonding interactions.² This study put forth a straightforward protocol to develop biologically relevant fluoroalkyl bis-indoles in a sustainable fashion through indepth insights gained from extensive DFT predictions. Furthermore, our latest study unfurls the crucial role of NCIs in electrochemical synthesis of unsymmetrically substituted NH-pyrroles from enamines.³ Trifluoroethanol additives are found to have "magical effect" on tuning oxidation potential of enamines through H-bonding and C-H $\cdots\pi$ interactions, thus facilitating the desired chemo-selective cross-coupling. Lastly, we discuss how NCIs underpin chirality in bifunctional squaramide catalyzed reactions leading to skeletal diversity in synthesis of azocine derivatives.⁴

References

- 1. H. J. Davis, R. J. Phipps, Chem. Sci. 2017, 8, 864 877.
- 2. V. Arun, L. Roy, S. De Sarkar, Chem. Eur. J. 2020, 26, 16649 16654.
- 3. M. Baidya, D. Maiti, L. Roy, S. De Sarkar, Angew. Chem. Int. Ed. 2022, 61, e202111679.
- 4. R. Khuntia, S. K. Mahapatra, L. Roy, S. C. Pan, Chem. Sci. 2023 (in revision)



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Lisa Roy received her B.Sc. and M.Sc. degrees in chemistry from the University of Calcutta, India in 2007 and 2009 respectively. Thereafter, she joined the group of Prof. Ankan Paul at the Indian Association for the Cultivation of Science, where she obtained her PhD degree in 2015. Subsequently, she worked as a postdoctoral researcher in the Molecular Theory and Spectroscopy research-group led by Prof. Frank Neese, under the guidance of Prof. Shengfa Ye, at the Max Planck Institute for Chemical Energy Conversion, Germany. She received the Department of Science and Technology, India, Inspire Faculty Award in 2017 and worked as an independent scientist at CSIR Central Mechanical Engineering Research Institute from 2017-18. Presently, she is working as an Assistant Professor at Institute of Chemical Technology - IOC Bhubaneswar campus. Her current research interests include bio-inspired homogeneous catalytic reactions, small molecule activations and utilization of non-covalent interactions for sustainable energy and resources.



FL-7

10-13 December 2023

Carbene-Supported Monoatomic Phosphorus Anion: An Excellent Ligand for Stabilization of Coinage Meal Nano-Clusters Exhibiting Thermally Activated Delayed Fluorescence; A Novel Photocatalyst at the Doorstep

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Applications of structurally well-defined coinage-metal nano-clusters (NCs) as optoelectronic materials, and homogeneous catalysts have been majorly restricted due to the inherent lower stability of such species. We have developed an efficient route for the syntheses of three robust and atomically precise coinage-metal(I) NCs stabilized by utilizing cyclic alkyl(amino) carbene (cAAC)-anchored monoatomic phosphorus anion (cAAC=P⁻).¹ Apart from the attractive metallophilic interactions [M---M; M = Cu, Ag], the enhanced kinetic, and thermodynamic stability of these NCs can be attributed to the excellent π accepting property of cAAC=P⁻ surrounding the metallic cores. The cAAC=P⁻ anion has been generated either in situ by anion-induced cleavage of the P-Sb/B bonds² of the corresponding stibanyl/boryl phosphaalkenes in presence of various coinage-metal(I)-CI/OTf/NTf2; or by directly introducing the alkali-metal phosphinidenide.³ Structural elucidations of all NCs have been established by NMR, ESI-MS, and single-crystal X-ray diffraction. The photoluminescence (PL) spectra of these NCs in solid state and in solution exhibited intense red to yellow to orange emissions, and high photoluminescence quantum yield (PLQY, Φ_{PL}) of up to 20% at room temperature with considerably higher average lifetimes (τ) of 26.3, 60.48, and 5.26 µs, respectively, indicative of the thermal equilibrium between the triplet excited state (T_1) and the lowest energy singlet excited state (S_1) . The observed red shift of the emission maxima in the temperature-dependent PL spectra within a temperature range of 300-80 K, and the smaller $\Delta E(S_1-T_1)$ values confirm the thermally activated delayed fluorescence (TADF) nature of all the reported NCs herein. Moreover, exploiting the TADF nature of the redox active Cu(I)₈ NC, it has been successfully employed as the first cAACphosphinidenide-based photocatalyst under blue LED at ambient condition for the diastereoselective cyclopropanation of substituted indoles/styrenes in excellent yields.

References

1. E. Nag, S. Battuluri, K. C. Mondal and S. Roy, *Chem. Eur. J.*, 2022, **28**, e202202324A.

2. E. Nag, S. Battuluri, B. B. Sinu and S. Roy, Inorg. Chem., 2022, 61, 13007-13014.

3. A. Kulkarni, S. Arumugam, M. Francis, P. G. Reddy, E. Nag, S. M. N. V. T. Gorantla, K. C. Mondal and S. Roy, *Chem. Eur. J.*, 2021, **27**, 200-20



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Dr. Sudipta Roy obtained her Ph.D. in Organic Chemistry as a DAAD Scholar from the Institute of Organic Chemistry at University of Regensburg, Germany in 2012, working on *Development of Novel Methodologies for the Syntheses of Biologically Relevant Nitrogen-Heterocycles* in the group of Prof. Dr. Oliver Reiser. In February 2013, she moved to the Institute of Organic and Biomolecular Chemistry at Georg-August-Universität Göttingen, Germany as a Postdoctoral Fellow, where she worked with Prof. Dr. Lutz Ackermann on *C-H, and C-N bond Activation using Cyclic Alkyl(Amino) Carbene (cAAC)-Stabilized Low Valence Transition Metal Complexes*. In 2014, she moved to the Institute of Inorganic Chemistry at Georg-August-Universität Göttingen, Germany as the Postdoctoral Fellow to work with Prof. Dr. Herbert W. Roesky, where she explored the *Fascinating Chemistry of Low Valence*, *Low Coordinate Group 14/15 Elements*. Currently, she is an Assistant Professor at Indian Institute of Science Education Research (IISER) Tirupati. Her Research Group focuses on *Carbene-Phosphinidenide-Stabilized Main Group Materials and Organic Homogeneous Catalysis*.



FL-8

10-13 December 2023

Aromatic Hydroxylations Catalysed by Nickel(II) Complexes of Pentadentate Ligands

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Targeting selective one-step oxidation of arenes under mild conditions has become a challenging and exciting scientific area that has drawn larger attention in recent years; because naturally available oxygenase enzymes efficiently and selectively perform such transformations under normal atmospheric conditions.¹ Inspired by naturally occurring oxygenase enzymes, numerous attempts to catalyze the oxidation of arenes using first-row transition metal catalysts have been made.^{1,2} Thus, we have designed, synthesized and characterized the series of pentadentate ligands, and isolated their nickel(II) complexes to investigate the catalytic ability toward aromatic substrates. The complexes show better catalytic activity with a good selectivity in arene oxidations and the results will be discussed during the presentation.

References

1. (a) A. Rajeev, M. Balamurugan and M. Sankaralingam, *ACS Catal.* **2022**, *12*, 9953-9982; (b) M. Sankaralingam, M. Balamurugan and M. Palaniandavar, *Coord. Chem. Rev.* **2020**, *403*, 213085.

2. (a) E. Kimura, R. Machida, J. Chem. Soc., Chem.Commun.**1984**, 499-500. (b) Y. Morimoto, S. Bunno, N. Fujieda, H. Sugimoto and S. Itoh, J. Am. Chem. Soc. **2015**, 137, 5867–5870. (c) S. Muthuramalingam, K. Anandababu, M. Velusamy, and R. Mayilmurugan, Catal. Sci. Technol. **2019**, 9, 5991-6001. (d) E. Masferrer-Rius, M. Borrell, M. Lutz, M. Costas and R. J. M. K. Gebbink, Adv. Synth. Catal. **2021**, 363, 3783–3795.



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FL-8

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Muniyandi Sankaralingam received his M.Sc. (2008) degree from ANJA College affiliated with Madurai Kamaraj University and completed PhD (2014) in Bioinorganic Chemistry from Bharathidasan University, Tiruchirappalli under the supervision of Prof. M. Palaniandavar. In 2014, he moved to EWHA Womans University, Seoul, South Korea to work with Prof. Wonwoo Nam and Prof. Shunichi Fukuzumi as a postdoctoral researcher and spent 4.4 years. He joined the National Institute of Technology Calicut, Kozhikode as an Assistant Professor in 2018 to start his independent career. His research group is currently focusing on Bioinspired and Biomimetic Chemistry Research by 'Designing and synthesizing the earth-abundant transition metal catalysts for clean energy, organic transformations and health sciences. He has received the Guest-Researcher Award from the University Paris City, France 2022 and the DST-INSPIRE Faculty Award 2018.

Representative publications:

- 1. M. Sankaralingam, Y.-M. Lee, W. Nam and S. Fukuzumi, *Coord. Chem. Rev.* **2018**, *365*, 41-59.
- 2. M. Sankaralingam, Y.-M. Lee, D. G. Karmalkar, W. Nam and S. Fukuzumi, J. *Am. Chem. Soc.* **2018**, *140*, 12695-12699.
- M. Sankaralingam, Y.-M. Lee, Y. Pineda-Galven, D. G. Karmalkar, M. S. Seo, S. H. Jeon, Y. N. Pushkar, S. Fukuzumi and W. Nam, *J. Am. Chem. Soc.* 2019, 141, 1324-1336.
- 4. M. Sankaralingam, M. Balamurugan and M. Palaniandavar, *Coord. Chem. Rev.* **2020**, *403*, 213085.
- 5. A. Rajeev, M. Balamurugan and M. Sankaralingam, *ACS Catal.* **2022**, *12*, 9953–9982.
- 6. A. Das, R. Sangavi, S. Gowrishankar, R. Kumar and M. Sankaralingam, *Inorg. Chem.* **2023**, *62*, 18926–18939.



10-13 December 2023

Transition-Metal-Catalyzed Allylic and Benzylic C-H Functionalization Reactions

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Transition-metal-catalyzed functionalization of relatively dormant C(sp³)-H bonds have gained profound importance as it proves to be a powerful strategy to enable C–C and C–heteroatom bond formation in a highly atom- and stepeconomical manner. In this context, allylic and benzylic C(sp³)-H bonds have gained particular attention since it can be utilized as a starting material for the synthesis of a wide range of organic chemical building blocks. The direct allylic C-H functionalization is an efficient method to avoid the functional group manipulations classically needed to obtain peroxidised substrates. Palladium catalysts have proven to be an efficient catalyst for linear selective allylic C-H functionalization of terminal alkenes. Recently, Rh(III) and Ir(III) complexes have been emerged as better alternative to achieve branch selectivity of terminal olefins as well as for the allylic C-H bond functionalization of internal alkenes.¹ In parallel, catalytic annulation via double C-H activation is now recognized as one of the most attractive methods to construct complex frameworks. This protocol enables the formation of multiple bonds in one pot, making it more atom- and stepeconomical compared to available methods. It will be impressive for carrying out annulation reactions that proceed via the activation of both a primary benzylic C–H bond and a meta C–H bond by using a weak directing group. In this talk, I would like to present our observation on transition-metal-catalysed direct allylic C-H functionalization of unactivated alkenes with various coupling partners and annulation reaction via dual C–H activation.³



References

(a) R. Giri, B. F. Shi, K. M. Engle, N. Maugel, J. Q. Yu, *Chem. Soc. Rev.*, 2009, **38**, 3242.
 (b) R. Manoharan, M. Jeganmohan, *Eur. J. Org. Chem.*, 2020, 7304.

2. (a) P. Sihag, M. Jeganmohan, *J. Org. Chem.*, 2019, **84**, 13053. (b) P. Sihag, M. Jeganmohan, *Chem. Commun.*, 2021, **57**, 6428. (c) P. Sihag, T. Chakraborty, M. Jeganmohan, *Org. Lett.*, 2023, **25**, 1257. (d) G. Naskar, M. Jeganmohan, *Chem. Eur. J.* 2022, **28**, e2022007. (e) G. Naskar, M. Jeganmohan, *Org. Lett.*, 2023, **25**, 2190.



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Prof. M. Jeganmohan received his master's degree in organic chemistry from the University of Madras in 2001. He earned his Ph.D. in 2005 from the National Tsing Hua University, Taiwan, under the guidance of Prof. Chien-Hong Cheng, and then pursued postdoctoral work in the same laboratory (2005–2009). He subsequently moved to the Ludwig-Maximilians-Universitat, Munich, Germany, to undertake post-doctoral studies, supported by the Alexander von Humboldt foundation, with Prof. Paul Knochel (2009 to 2010).

Research Interests: Metal-catalyzed organic reactions, Natural products synthesis and Asymmetric synthesis

Awards and Honours:

- 1. 2022, Chemical Research Society of India (CRSI) Bronze Medal
- 2. 2021, Fellow of the Academy of Sciences, Chennai
- 3. 2021-2022, Fellow under "The (Late) Shri. G. D. Gokhale Lectureship Endowment", Institute of Chemical Technology (ICT), Mumbai
- 4. 2019, Fellow Royal Society of Chemistry (FRSC)
- 5. 2014, ISCB Award of Appreciation for Chemical Science, CSIR-CDRI Lucknow
- 2013, Alkyl Amines ICT Young Scientist Award by Institute of Chemical Technology Mumbai, India
- 7. 2013, 2013: Science Academy Medal for Young Scientists, Indian National Science Academy, New Delhi, India
- 8. 2012 2015, Science Academy Medal for a young associate, Indian Academy of Sciences, Bangalore, India.
- 9. September 2011, DAE Young Scientist Research Award, BRNS, BARC, India.

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- 1. July 2021 Till now, Professor, IIT Madras
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IL-28

10-13 December 2023

Molecular defined manganese catalysts for hydrogenation reactions

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The development of non-noble metal-based catalytic systems has been increasing since the beginning of the century, notably in the field of reduction or hydroelementation reactions. Significant progress has been accomplished with catalysts based on iron and cobalt. Manganese is the third most abundant metal in the Earth's crust (after iron and titanium). Its biocompatibility as well as its availability and low cost are undeniable assets for the development of catalytic systems of societal and environmental interest. Surprisingly, its use as an alternative to noble metals in hydrogenation and related reactions had not been considered prior to the work of Beller in 2016.^[1] From then on, examples of reduction reactions catalyzed by well-defined manganese complexes have flourished in the literature.^[2] Our group has contributed to the field with the development of Mn-based catalytic systems relying on metal-ligand cooperation for the hydrogenation (with H₂ or *i*PrOH) of polar bonds.^[3] In this context, the recent results obtained in ester hydrogenation will be presented more in detail.



References

1. S. Elangovan, C. Topf, S. Fischer, H. Jiao, A. Spannenberg, W. Baumann, R. Ludwig, K. Junge, M. Beller, *J. Am. Chem. Soc.* **2016**, *138*, 8809-8814.

2. Manganese Catalysis in Organic Synthesis, J.-B. Sortais (Ed.), Wiley-VCH Verlag GmbH, 2021.

3. a) A. Bruneau-Voisine, D. Wang, V. Dorcet, T. Roisnel, C. Darcel, J.-B. Sortais, *Org. Lett.* **2017**, *19*, 3656-3659; b) R. Buhaibeh, O. A. Filippov, A. Bruneau-Voisine, J. Willot, C. Duhayon, D. A. Valyaev, N. Lugan, Y. Canac, J.-B. Sortais, *Angew. Chem. Int. Ed.* **2019**, *58*, 6727-673; c). K. Azouzi, L. Pedussaut, R. Pointis, A. Bonfiglio, R. Kumari Riddhi, C. Duhayon, S. Bastin, J.-B. Sortais, *Organometallics* **2023** DOI: 10.1021/acs.organomet.3c00137



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Jean-Baptiste Sortais is professor at the Paul Sabatier University in Toulouse (France) and conducts his research work on homogeneous organometallic catalysis within a laboratory of the French National Research Centre (CNRS) - the Laboratory for Coordination Chemistry (LCC).

Jean-Baptiste Sortais obtained a DEA graduate degree (Master 2), then a PhD at the University of Strasbourg (then Louis Pasteur University) under the supervision of Dr. Michel Pfeffer. His research work focused on the synthesis of chiral cyclometallated complexes of ruthenium and their applications in catalysis. He subsequently carried out two post-doctoral stays; with Professor Jan-Erling Bäckvall at the University of Stockholm (Sweden) on dynamic kinetic resolution, then with Professor Gerhard Erker at the University of Münster (Germany) in the field of Lewis-Frustrated pairs. In 2009, he was recruited as associate professor within the team Organometallics: Materials and Catalysis at the Rennes Institute of Chemical Sciences (ISCR) of the University of Rennes 1. In 2017, he was promoted to full professor at the Paul Sabatier University in Toulouse.

His current research work is mainly focused on the development of new molecular catalysts based on abundant 3d transition metals, such as iron, nickel, cobalt, and manganese. Catalytic applications focus on reduction processes in the broad sense (hydroelementation, hydrogenation, dehydrogenation, hydrogen transfer, hydrosilylation, hydroboration and hydrogen borrowing) and direct activation of C-H bonds. The main objective of his work is thus to promote new reactivities and/or selectivities based on readily available and inexpensive metal catalysts in the context of sustainable chemistry.

In 2016, he was appointed Junior Member of the Institut Universitaire de France (IUF) and received the 2019 Young Researcher Award from the Catalysis Division of the French Chemistry Society (SCF).



IL-29

10-13 December 2023

Breaking Symmetry: Challenges & Opportunities

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Human minds are fascinated by symmetrical objects, and we admire the challenges in constructing symmetrical architectures whenever we find one around us. In contrast to the physical world, we live in, creating symmetry in the molecular world is a relatively simple task. It is the daunting asymmetry in molecules that often challenges the chemists.

Breaking symmetry to generate asymmetry, commonly termed as *desymmetrization*, is a remarkably powerful strategy for building molecular complexity. Successful implementation of this strategy holds the potential to forge multiple stereogenic centers in a single step. In fact, stereocenters can also be created away from the reaction site.

During the past few years, we have developed a number of organocatalytic enantioselective desymmetrization reactions¹ from formal $C(sp^2)$ –H alkylations² and alkenylation³ to the *de novo* construction of arenes⁴ and heteroarenes.⁵ The topic of this talk will be primarily confined to these enantioselective desymmetrization reactions and their applications for the synthesis of complex targets.⁶

References

- 1. (a) Singha Roy, S. J.; Mukherjee, S. *Chem. Commun.* **2014**, *50*, 121. (b) Manna, M. S.; Mukherjee, S. *Chem. Sci.* **2014**, *5*, 1627.
- (a) Manna, M. S.; Mukherjee, S. J. Am. Chem. Soc. 2015, 137, 130. (b) Sarkar, R.; Mukherjee, S. Org. Lett. 2016, 18, 6160. (c) Mallojjala, S. C.; Sarkar, R.; Karugu, R. W.; Manna, M. S.; Ray, S.; Mukherjee, S.; Hirschi, J. S. J. Am. Chem. Soc. 2022, 144, 17399.
- 3. Manna, M. S.; Sarkar, R.; Mukherjee, S. Chem.-Eur. J. 2016, 22, 14912.
- 4. Ghosh, B.; Harariya, M. S.; Mukherjee, S. Angew. Chem. Int. Ed. 2022, 61, e202204523.
- 5. Ghosh, B.; Balhara, R.; Jindal, G.; Mukherjee, S. Angew. Chem. Int. Ed. 2021, 60, 9086.
- 6. Ray, S.; Mondal, S.; Mukherjee, S. Angew. Chem. Int. Ed. 2022, 61, e202201584.



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Santanu obtained his B.Sc. (Chemistry Hons.) from Ramakrishna Mission Residential College, Narendrapur (2000) and M.Sc. (Chemistry) from Indian Institute of Technology, Kanpur (2002). After earning his Ph.D. (*summa cum laude*) in 2006 working with Professor Albrecht Berkessel at Universität zu Köln, Germany, he worked as a postdoctoral fellow with Professor Benjamin List at Max-Planck Institut für Kohlenforschung in Mülheim an der Ruhr, Germany (2006-2008) and with Professor E. J. Corey at Harvard University, USA (2008-2010). In 2010, he returned to India to take up an Assistant Professor position at the Department of Organic Chemistry in Indian Institute of Science, Bangalore. He was promoted to Associate Professor in 2015 and Professor in 2021.

Santanu's research interests revolve around various aspects of asymmetric catalysis, with a particular emphasis on desymmetrization and remote stereocontrol using different classes of organocatalysts. In addition, his research group is also works on transition metal-catalyzed enantioselective allylic, allenylic and propargylic substitution reactions.

Santanu is a recipient of the Thieme Chemistry Journals Award (2011), the Indian National Science Academy (INSA) Medal for Young Scientist (2014), Chemical Research Society of India (CRSI) Bronze Medal (2019), A. V. Rama Rao (AVRA) Young Scientist Award for the year 2019 and the Science and Technology Award for Research by Science and Engineering Research Board (SERB-STAR) for the year 2021. In 2018, he became a Fellow of the Royal Society of Chemistry, London (FRSC). He is an Associate Editor of *Organic & Biomolecular Chemistry* (RSC) and a member of the Editorial Advisory Board of the *Journal of Organic Chemistry* (ACS), and *SYNLETT* (Thieme).



10-13 December 2023

IL-30

Enantioselective Copper-Catalyzed Reductive Coupling of Alkoxyallenes

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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. Here, we have developed the Cu(I)-catalyzed enantioselective synthesis of complex 1,2-*synsec,tert*-diols and α -hydroxy ketones using reductive coupling of alkoxy-allenes with carbonyl compounds.



References

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.



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Rambabu Chegondi received his M.Sc. (2003) degree from University of Hyderabad and completed Ph.D. (2009) in Organic Synthesis from Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad under the supervision of Dr. S. Chandrasekhar. In 2009, he moved to The University of Kansas, USA to work with Prof. Paul R. Hanson as a postdoctoral researcher. He joined CSIR-IICT, Hyderabad as CSIR-Pool-Scientist (SRA) in 2014 as an independent researcher. He is currently a Principal Scientist at the OS&PC department, CSIR-IICT, focusing on the development of new enantioselective desymmetrization methodologies and new process development of key APIs. He has received the Eli Lilly Asia Best Thesis Award 2009, AVRA-Young Scientist Award-2019, Thieme Chemistry Journals Award, and SERB-STAR Award. He is an FRSC and currently an Editorial Advisory Board Member of Organic Letters.



IL-31

10-13 December 2023

Oxidations with IBX: Progression to Heterogeneous Catalysis

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We consider 'molecular structure as an embodiment of organic reactivity as well as macroscopic bulk property'. By dealing with structural attributes at the molecular level, it is possible to control organic reactivity as well as the properties of macroscopic solids. I will exemplify control of molecular reactivity for the development of catalytic materials.

IBX, *o*-iodoxybenzoic acid, has emerged as an indispensable oxidation reagent in contemporary organic oxidation chemistry. Its progression from being an ignored material for close to a century on account of its reprehensible insolubility to the present-day application as a catalyst in the presence of a terminal oxidant such as Oxone constitutes a remarkable development. I will present our endeavours focused on the development of IBX-precatalysts.¹ As a logical extension of these studies, I will demonstrate our bottom-up approach toward the development of tailor-made heterogeneous IBX pre-catalysts for oxidations based on porous organic polymer (POPs), emergent materials.³ The construction of functional porous metal-organic materials in a bottom-up molecules-to-materials fashion continues to be one of our hot research pursuits.³

References

- J. N. Moorthy, J. N.; K. Senapati, K. N. Parida, S. Jhulki, K. Sooraj, and N. N. Nair, J. Org. Chem. 2011, 76, 9593. b) S.Seth, S. Jhulki, J. N. Moorthy, Eur. J. Org. Chem. 2013, 2445. c) J. N. Moorthy, and K. N. Parida, J. Org. Chem. 2014, 79, 11431. d) A. K. Mishra and J. N. Moorthy, Org. Chem. Front. 2017, 04, 343. e) K. N. Parida, J. N. Moorthy, Synlett 2023, 34, 495. f) K. N. Parida, J. N. Moorthy, Chem. Eur. J. 2023, 29, e202203997.
- a) Yadav, C.; Maka, V. K.; Payra, S.; Moorthy, J. N. *J. Catal.* 2020, *384*, 61. b) C. Yadav, V. Maka, S. Payra, J. N. Moorthy, ACS Applied Poly. Materials 2020, *2*, 3084, c) C. Yadav, A. K. Sahoo, J. N. Moorthy, *ACS Appl. Nanomater.* 2022, *5*, 14296. d) C. Yadav, S. Payra, J. N. Moorthy, *J. Catal.* 2022, *414*, 769. e) K. Alka, J. N. Moorthy, *ChemCatChem* (2023).
- P. Chandrasekhar, A. Mukhopadhyay, G. Savitha, J. N. Moorthy, *Chem. Sci.* 2016, 07, 3085.
 b) P. Chandrasekhar, A. Mukhopadhyay, G. Savitha, J. N. Moorthy, *J. Mater. Chem. A.* 2017, 5, 5402.
 c) A. Mukhopadhyay, V. Maka, G. Savitha, J. N. Moorthy, *Chem* (Cell Press), 2018, 4, 1069.
 f) Maka, V. K.; Tamuly, P.; Jindal, S.; Moorthy, J. N. App. Mater. Today 2020, 19, 100613.



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Dr. J. N. Moorthy obtained Ph.D degree from the Organic Chemistry Department of the Indian Institute of Science, Bangalore in 1994. He pursued postdoctoral research in the University of Houston, USA, the University of Wuerzburg, Germany and the University of Victoria, Canada prior to joining the Chemistry Department, IIT Kharagpur in 1998. After a 5-month stint, he moved to IIT Kanpur. He has been a full professor at IITK since 2008. He moved to IISER Thiruvananthapuram as the Director in April 2019.

He is a recipient of AvH postdoctoral research fellowship in Germany (1995-96), a young chemist award, and bronze and silver medals from the Chemical Research Society of India (CRSI), India. He received the Shanti Swarup Bhatnagar Prize in Chemical Sciences, India (2008), and the Sastra-CNR Rao Award in Chemical Sciences (2020). He is a Fellow of the Indian Academy of Sciences Bangalore (2010), a Fellow of the Royal Society of Chemistry (2014) and a Fellow of the Indian National Science Academy (2018). He has also been a J. C. Bose National Fellow since 2015. He has been on the editorial boards of New J. Chemistry, J. Chem. Sci. and Int. J. Photoenergy. He is presently an associate editor of J. Chem. Sci.

His interests are in the areas of supramolecular chemistry, organic materials, mechanistic organic chemistry and organic photochemistry.



IL-32

10-13 December 2023

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

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N-Heterocyclic carbene (NHC)-catalyzed umpolung of aldehydes is widely used for the unconventional access to target molecules.¹ Although the assembly of axially chiral C-C bonds leading to the atroposelective synthesis of biaryls and related compounds are well-known, the analogous synthesis of compounds bearing axially chiral C-Heteroatom bonds are relatively rare using NHC catalysis. We have recently reported the NHC-catalyzed atroposelective synthesis of N-aryl succinimides having an axially chiral C-N bond via the desymmetrization of N-aryl maleimides.² Moreover, we have demonstrated the NHC-catalyzed kinetic resolution of N-aryl aminomaleimides allowing the synthesis of C-N axially chiral N-aryl aminomaleimides via remote chirality control.³ In addition, NHC-catalyzed selective amidation reaction leading to the atroposelective synthesis of N-N axially chiral 3-amino quinazolinones has been realized recently.⁴ Further, we have uncovered the NHC-catalyzed synthesis of C-O axially chiral diaryl ethers via atroposelective esterification of dialdehyde-containing diaryl ethers via a desymmetrization strategy.⁵ The details of these works will be presented.



References

- For reviews, see: (a) Flanigan, D. M.; Romanov-Michailidis, F.; White, N. A. Rovis, T. Chem. Rev. 2015, 115, 9307. (b) Enders, D.; Niemeier, O.; Henseler, A. Chem. Rev. 2007, 107, 5606. For a Book, see: (c) Biju, A. T. N-Heterocyclic Carbenes in Organocatalysis; Wiley-VCH Verlag GmbH & Co. KGa A: Boschstr. 12, 69469 Weinheim, Germany, 2019.
- 2. Barik, S.; Shee, S.; Das, S.; Gonnade, R. G.; Jindal, G.; Mukherjee, S.; Biju, A. T. Angew. Chem. Int. Ed. **2021**, 60, 12264.
- 3. Barik, S.; Das, R. C.; Balanna, K.; Biju, A. T. Org. Lett. 2022, 24, 5456.
- Balanna, K.; Barik, S.; Barik, S.; Shee, S.; Manoj, N.; Gonnade, R. G.; Biju, A. T. ACS Catal. 2023, 13, 8752.
- 5. Shee, S.; Ranganathappa, S. S.; Gadhave, M. S.; Gogoi, R.; Biju, A. T. *ChemRxiv*. **2023**, Preprint. <u>https://doi.org/10.26434/chemrxiv-2023-km9t7</u>



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SL-7

10-13 December 2023

A tale of two enzymes: Iron catalysis in enzymes that break the C-N bond

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Transition metal ions play a vital role in the redox chemistry of enzymes. In this talk, I will demonstrate how iron chemistry is used for redox and amide hydrolysis in bacterial enzymes. In the enzyme dimethylformamidase, a square pyramidal Fe (III) functions as a Lewis acid to hydrolyse a tough amide bond in N,N dimethylformamide. In dioxygenases, like trimethylamine monooxygenase or 3-nitro toluene dioxygenase, iron plays a redox-active role in breaking a C-N bond.



3-Nitrotoluene dioxygenase 5XBP



DMFase 6LVC



10-13 December 2023

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Gurunath did his PhD from the IISc., Bangalore, under the guidance of Prof. P. Balaram in peptide chemistry. He subsequently did his post-doctoral work at MIT, Cambridge, USA and Karolinska Institute, Sweden, before joining IIT Kanpur in 2000, where he is currently a senior professor. At IIT Kanpur, his research has focused on environmental biochemistry, particularly the environmental degradation of explosives and C-1 compounds. As luck would have it, nearly all enzymes worked on in his group have transition metals doing the catalysis. He has mentored over 20 PhD students and several master's students.



SL-8

10-13 December 2023

Photocatalyzed Dowd–Beckwith Radical-Polar Crossover Reaction for the Synthesis of Medium-Sized Carbocyclic Compounds

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The Dowd–Beckwith reaction, an effective strategy for synthesizing mediumsized carbocyclic compounds via alkoxy radicals induced ring-expansion of carbonyl compounds, which takes advantage of existing ring structures and avoids the entropic and enthalpic aspects associated with end-to-end cyclization pathways.¹ However, the predominant route remains the Dowd– Beckwith ring-expansion accompanied by H-atom abstraction, hampering its synthetic applications. Additionally, there are no existing reports on noncarbon nucleophilic reagents for functionalizing the ring-expanded radicals.² Herein, we present a redox-neutral decarboxylative Dowd–Beckwith/radicalpolar crossover (RPC) sequence. This strategy furnishes functionalized medium-sized carbocyclic compounds, accommodating various nucleophiles.³ The process facilitates one-carbon ring-expansion for 4-, 5-, 6-, 7-, and 8membered ring substrates. Furthermore, it can extend to incorporate threecarbon chains, enabling distant functionalization within medium-sized rings.



References

1. (a) A. L. J. Beckwith, D. M. O'Shea, S. Gerba and S. W. Westwood, *J. Chem. Soc., Chem. Commun.*, **1987**, 666-667. (b) P. Dowd and S. C. Choi, *J. Am. Chem. Soc.*, **1987**, *109*, 3493-3494.

2. T. Singha, A. Rouf Samim Mondal, S. Midya and D. P. Hari, *Chem. Eur. J.*, **2022**, *28*, e202202025.

3. T. Singha, G. A. Kadam and D. P. Hari, Chem. Sci., 2023, 14, 6930-6935.



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IL-33

10-13 December 2023

Sustainable Catalysis Enabled by Metal-Ligand Cooperation

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Construction of C-C and C-N bonds are important reactions in organic synthesis. Catalytic alkylation using alcohol as an alkylation reagent is a green alternative to the conventional alkylation reactions involving alkyl halides and stoichiometric reagents. Employing Ru-macho pincer catalyst which operates via amine-amide metal-ligand cooperation, simple and atom-economical direct alkylation of nitriles was attained. We have also discovered the catalytic cross-

of secondary coupling alcohols. a-Alkylation and aprenylation of ketones using secondary alcohols and prenol, respectively were reported. a-Alkylation of bnaphthols using primary alcohols reported was recently. Catalvtic formal conjugate addition of nitriles with allylic alcohols was developed. Using secondary alcohols, a-alkenylation of nitriles synthesis of and ketazine were also reported. Remarkably, water and liberated molecular hydrogen are the only byproducts in these reactions making these



Scheme 1. Green catalysis by Ru-MACHO catalyst.

catalytic transformations environmentally benign.

References

- 1. Thiyagarajan, S.; Gunanathan, C. ACS Catal. 2017, 7, 5483-5490.
- 2. Thiyagarajan, S.; Gunanathan, C. ACS Catal. 2018, 8, 2473-2478.
- 3. Kishore, J.; Thiyagarajan, S.; Gunanathan, C. Chem. Commun. 2019, 55, 4542-4545.
- 4. Thiyagarajan, S.; Gunanathan, C. J. Am. Chem. Soc. 2019, 141, 3822-3827.
- 5. Thiyagarajan, S.; Gunanathan, C. Synlett 2019, 30, 2027-2034. (Invited Synpacts article).
- 6. Thiyagarajan, S.; Gunanathan, C. Org. Lett. 2020, 22, 6617-6622.
- 7. Thiyagarajan, S.; Vijaya Sankar, R. Gunanathan, C. Org. Lett. 2020, 22, 7879-7884.
- 8. Thiyagarajan, S.; Gunanathan, C. Org. Lett. 2019, 21, 9774-9778.

9. Thiyagarajan, S.; Vijaya Sankar, R.; Anjalikrishna, P. K.; Suresh, C. H.; Gunanathan, C. ACS Catal. **2022**, *12*, 2191-2204.

10. Vijaya Sankar, R.; Manikpuri, D.; Gunanathan, C. Org. Biomol. Chem. 2023, 21, 273-278.

11. Vijaya Sankar, R.; Mathew, A.; Pradhan, S; Kuniyil, R.; Gunanathan, C. *Chem. Eur. J.* **2023**, e202302102.

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- 2011 Assistant Professor, NISER Bhubaneswar, India
- 2011 Ramanujan Fellow (SERB), NISER Bhubaneswar, India
- 2009 AvH Research Fellow, RWTH Aachen University, Germany
- 2006 Dean of Faculty Postdoctoral Fellow, Weizmann Institute of Science, Israel
- 2005 Postdoctoral Fellow, Weizmann Institute of Science, Israel

Education

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

Awards

- 2020 Top 3% highly cited author from India in ACS
- 2020 Thieme Chemistry Journals Award
- 2020 CRSI Bronze medal
- 2019 Top Peer Reviewer Award by Publons
- 2016 ECRP award -First Prize (10,000 Euro).
- 2011 Ramanujan Fellowship. SERB, New Delhi.

Research Interests: Catalysis

Organometallic Chemistry Reaction mechanism, and Synthetic methods.



IL-34

10-13 December 2023

Visible-Light-Fueled Catalysis involving Energy and Electron Transfer

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Rapid generation of molecular complexity from readily available starting materials is one of the trickiest approaches in synthetic chemistry. Visible-light photocatalysis has emerged as an effective tool for such purposes.¹ Upon excitation by a visible-light photon, a photosensitizer can engage in a number of productive bimolecular reactions. A Dexter energy transfer (EnT) can directly excite an organic substrate to its triplet state. The application of such a process for dearomative cycloaddition reactions will be shown.² Besides, the excited state of the photocatalyst can also engage in electron transfer reactions. The application of such reactions for producing low-valent cobalt³ and nickel⁴ complexes will be shown. The control generation of these highly reactive and sensitive species enabled diverse coupling reactions in high yields with high control of relative and absolute stereochemistries. Finally, the presentation will discuss the effect of proximity and interlocking in these dual catalytic systems for visible light-fueled cross-coupling reactions.⁵



References

1. W. C. MacMillan et al. Chem. Rev. 2022, 122, 1485

2. P. Rai, † K. Maji, S. K. Jana, B. Maji, Chem. Sci. 2022, 13, 12503.

3. (a) P. Rai, K. Maji, B. Maji; *Org. Lett.* **2019**, *21*, 3755; (b) K. Maji, P. R. Thorve, P. Rai, B. Maji, *Chem. Commun.* **2022**, *58*, 9516; (c) M. Maiti, S. K. Jana, B. Maji, *Chem. Commun.* **2023**, *59*, DOI: d3cc02792a.

4. (a) S. K. Jana, M. Maiti, P. Dey, B. Maji, *Org. Lett.* **2022**, *24*, 1298; (b) P. Dey, S. K. Jana, P. Rai, B. Maji, *Org. Lett.* **2022**, *24*, 6261.

5 (a) A. Jati, K. Dey, M. Nurhuda, M. Addicoat, R. Banerjee, B. Maji, *J. Am. Chem. Soc.* **2022**, *144*, 7822-7833; (b) A. Jati, S. Dam, S. Kumar, K. Kumar, B. Maji, *Chem. Sci.* **2023**, *14*, DOI: D3SC02440G.



10-13 December 2023

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1987: Born, Howrah, India

2007: B.Sc. University of Calcutta (Chemistry Hons.)

2009: M.Sc. Indian Institute of Technology Kanpur (Chemistry)

2012: PhD Ludwig Maximillan Universität Munich, Supervisor: Prof. Herbert Mayr

2013-2015: Postdoc: Chubu University, Mentor: Prof. Hisashi Yamamoto

2016: Alexander von Humboldt fellow: Westfälische Wilhelms-Universität Münster, Mentor: Prof. Frank Glorius

2016-2021: Assistant Professor, Indian Institute of Science Education and Research Kolkata

2021-: Associate Professor, Indian Institute of Science Education and Research Kolkata

Research focus: Organic synthesis, catalysis, and mechanistic studies.

Awards:

2021: "2021 Young Investigator Award ", Sponsored by Molecules

2021: Merck Young Scientist Award (runner-up) in Chemical Science

2021: INSA Medal for Young Scientists

2021: Associate of the Indian Academy of Sciences (IASc)

2020: NASI-Young Scientist Platinum Jubilee Award (2020) in Chemical Sciences

2019: Thieme Journal Award

Selected publication:

- A. Jati, S. Dam, S. Kumar, K. Kumar, **B. Maji**, *Chem. Sci.* **2023**, *14*, doi: 10.1039/D3SC02440G.
- S. Waiba, K. Maji, M. Maiti, B. Maji, *Angew. Chem. Int. Ed.* **2023**, *Angew. Chem. Int. Ed.* **2023**, 62, e202218329.
- P. Rai, K. Maji, S. K. Jana, B. Maji, *Chem. Sci.* **2022**, *13*, 12503-12510.
- K. Das, S. Waiba, A. Jana, B. Maji, Chem. Soc. Rev. 2022, 51, 4386-4464.
- A. Jati, K. Dey, M. Nurhuda, M. A. Addicoat, R. Banerjee, B. Maji, J. Am. Chem. Soc. **2022**, 144, 7822-7833.
- S. Waiba, M. Maiti, B. Maji, ACS Catalysis 2022, 12, 3995-4001.
- S. K. Jana, M. Maiti, P. Dey, B. Maji, Org. Lett. 2022, 24, 1298-1302.
- K. Das, K. Sarkar, B. Maji, ACS. Catal. 2021, 11, 7060-7069.
- K. Sarkar, K. Das, A. Kundu, D. Adhikari, B. Maji, *ACS. Catal.* **2021**, *11*, 2786-2794.



SL-9

10-13 December 2023

Introducing RSC Sustainability and related RSC journals

Emma Eley Executive Editor, Royal Society of Chemistry



10-13 December 2023

Emma Eley

Executive Editor, Royal Society of Chemistry



Emma is Executive Editor at the Royal Society of Chemistry with responsibility for the Environmental Science, Energy, and Sustainability Gold Open Access journals (namely <u>Environmental Science: Advances</u>, <u>Environmental Science: Atmospheres</u>, <u>Energy Advances</u>, <u>EES Catalysis</u> and <u>RSC Sustainability</u>).

As Executive Editor she leads the Editorial team responsible for the operational, strategic, and development aspects of the journals, working closely with the journals' Editorial Boards and the wider research community. A big part of her job is to uphold excellent standards and ensure that the journals deliver the quality, impact and timeliness that RSC journals are well-known for. Emma has over 12 years' experience within the scientific publishing industry and has worked on a variety of different journals during this time, including RSC Advances, Green Chemistry, ESPI, ES:Nano, ES:WRT and many more. Prior to working in the publishing industry, Emma obtained her 1st class Masters degree in Chemistry from Cardiff University, Wales, UK.





10-13 December 2023

SL-10 Generation of *N*-Centered Radicals Under Visible Light Photoredox Catalysis

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Herein, we have disclosed C–N and C–C bond formation strategies via *N*-centered radicals. We have utilized easily synthesizable oxime-esters and iminoesters as the precursor under blue LED irradiation. Fluoroalkylation using Langlois reagent (CF₃SO₂Na) is a very common synthetic technique,^[1] we have exploited it for synthesizing pharmaceutically valuable trifluoroarylated amino acids **2**. In this case, reductive trifluoromethylation of α -iminoesters occurs via umpolung strategy to generate *N*–centred radical under photoredox catalysis, which rearranges to form *C*–centred radical followed by radical-radical coupling of trifluoromethyl radical delivering the desired trifluoromethylated product **2**.^[2]

On the other hand, oxime-esters have been used as the source of iminyl radicals.^[3] Photocycloaddition is an age-old process.^[4] Our another thoughtprocess combines these altogether to attain a cycloaddition of olefins followed by iminyl addition under photocatalyzed blue LEDs irradiation. Successfully we have discovered a multitasking Ir-catalysis combining both energy-transfer and photoredox process. α , α '-disubstituted olefins **3** generates the *E*-selective imine addition product **4**, while *Z*-selective aminated stilbene derivatives **6** are obtained using simple unsubstituted styrenes **5**.^[5]



Scheme 1: Photoredox mediated various reactivities of *N*-centred radicals.

References

- 1. (a) D. A. Nagib and D. W. C. MacMillan, *Nature*, 2011, **480**, 224–228. (b) J. Xie, X. Yuan, A. Abdukader, C. Zhu and J. Ma, *Org. Lett.*, 2014, **16**, 1768–1771.
- 2. H. Paul, S. K. Ariyan, S. Pradhan and I. Chatterjee (manuscript under preparation).
- (a) G. Tan, M. Das, H. Keum, P. Bellotti, C. Daniliuc and F. Glorius, *Nat. Chem.*, 2022, 14, 1174–1184. (b) S. -Q. Lai, B. -Y. Wei, J. -W. Wang, W. Yu and B. Han, *Angew. Chem.*, *Int. Ed.*, 2021, 60, 21997–22003.
- 4. S. Poplata, A. Tröster, Y. Q. Zou, and T. Bach, Chem. Rev., 2016, 116, 9748–9815.
- 5. B. Paul, S. Das and I. Chatterjee (manuscript under preparation).



10-13 December 2023

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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. After that 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. Since December 2016 he is holding a position of Assistant Professor at the Indian Institute of Technology Ropar, India.

Details of any fellowship/awards/honors

(i) National Scholarship in Secondary and Higher Secondary exam. (2000 & 2002).

(ii) Ph.D. scholarship of the International Graduate School of Chemistry (GSC-MS), University of Muenster, Germany (2008-2011)

(iii) Postdoctoral Fellowship at ICIQ, Tarragona, Spain (2012-2014)

(iv) Cluster of Excellence UniCat Fellowship for Postdoctoral Research at Technical University Berlin, Germany (2014-2016)

(v) Institute Best Teaching Award (2020).

(vi) Thieme Chemistry Journal Award, 2022.



FL-9

10-13 December 2023

Enantioselective ring opening of vinyl aziridines using ppm-level iridium catalysis

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Chiral β -amino alcohol is considered as a privileged motif, ubiquitous in natural products, medicinally important compounds and in catalysts. Chiral β -amino alcohols are also versatile intermediates for the synthesis of many useful organic compounds. An efficient atom-economic approach for a highly regioand enantioselective ring opening of vinyl aziridines using unactivated carboxylic acids as oxygen nucleophiles has been developed for the synthesis of β -amino alcohols. Parts per million (ppm) level catalyst loading can be used to induce high yield and enantioselectivity in the vicinal amino alcohol products. The practical utility of this method is demonstrated by the application of the products in useful transformations.



References

- 1. Adhikari, A. S.; Pandit, S.; Kant, R.; Majumdar, N. ACS Catal. 2023, 13, 6261–6267.
- 2. Majumdar, N. ACS Catal. 2022, 12, 8291-8324.
- 3. Pandit, S.; Adhikari, A. S.; Majumdar, N. Org. Lett. 2022, 24, 7388–7393.



10-13 December 2023

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Dr. Nilanjana Majumdar started her chemistry journey from Visva-Bharati University in West Bengal, India. She completed her undergraduate education there with 1st class 1st in B.Sc. (Chemistry Hons.). In 2003, she went to IIT Kharagpur to pursue Masters. For Ph.D., she moved to United States in 2006 and worked under the supervision of Professor William D. Wulff in Michigan State University. After graduation in 2012, she moved to Tokyo, Japan for first postdoctoral experience in Professor Masakatsu Shibasaki's group with JSPS fellowship. After three years in Japan, she worked in Professor Benjamin List's group for one year in Max-Planck Institut für Kohlenforschung, Germany. In April, 2018, she joined CSIR-Central Drug Research Institute (CSIR-CDRI), Lucknow as Senior Scientist in Medicinal & Process Chemistry Division. Her research interest is mainly focused on the asymmetric catalysis.



FL-10

10-13 December 2023

Catalytic C-C Bond Functionalization of Aliphatic Ketones

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Ketone functionality, ubiquitous in commodity chemicals, pharmaceuticals and natural products, is regarded as one of the versatile synthetic intermediates in organic synthesis.¹ Unlike conventional reactivity (e.g. nucleophilic addition to C=O, \Box C-H functionalization via enol/enolate), harnessing strong \Box C-C activation of ketone moiety is challenging.² Recently, the strategy of converting aliphatic ketone to dihydroquinazolinone that is susceptible to redox-activation for liberating alkyl radical via C-C cleavage, has emerged as an enabling technique for mild C-C functionalization.^{3,4} In this presentation, the effort towards the development of synthetic methods, using aliphatic ketones as alkyl surrogate, will be presented.⁴

References

1. D. J. Foley and H. Waldmann, *Chem. Soc. Rev.,* 2022, **51**, 4094.

2. Y. Xia and G. Dong, *Nat. Rev. Chem.*, 2020, **4**, 600. b) G. Fumagalli, S. Stanton and J. F. Bower, *Chem. Rev.*, 2017, **117**, 9404.

3. Selected reports: L. Li, L. Fang, W. Wu and J. Zhu, *Org. Lett.*, 2020, **22**, 5401. b) X. –Y. Lv, R. Abrams and R. Martin, *Angew. Chem. Int. Ed.*, 2023, **62**, e202217386. c) H. Wu, S. Chen, D. Xiao, F. Li, K. Zhou, X. Yin, C. Liu, X. He and Y. Shang, *Org. Lett.*, 2023, **25**, 1166.

P. P. Mondal, A. Pal, A. K. Prakash and B. Sahoo, *Chem. Commun.* 2022, **58**, 13202. b) P.
 P. Mondal, A. Pal, S. Das, S. M. Vijayan, A. V. Nair, S. Ojha and B. Sahoo, *Synlett*, 2023, **34**, 1241. c) P. P. Mondal, S. Das, S. Venugopalan, M. Krishnan and B. Sahoo, *Org. Lett.*, 2023, **25**, 1441. d) S. Bag, S. Ojha, S. Venugopalan and B. Sahoo, *J. Org. Chem.*, 2023, **88**, 12121.



10-13 December 2023

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Dr. Basudev Sahoo completed his BSc in chemistry from the Ramakrishna Mission Residential College, affiliated to the University of Calcutta in 2009 and MSc in Chemistry from the Indian Institute of Technology (IIT) Kanpur in 2011. Then, he moved to Germany to pursue his PhD under the supervision of Prof. Frank Glorius at the University of Muenster. After completing his PhD in 2015, he moved to the group of Prof. Matthias Beller at the Leibniz Institute for Catalysis (LIKAT), Rostock, Germany as a Leibniz Postdoctoral Fellow. In 2018, he received Marie Curie (MSCA) postdoctoral fellowship and joined the group of Prof. Ruben Martin at the Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain. Since March 2020, he is holding a position of assistant professor in the school of chemistry Journals Award 2022 from the Thieme Verlag, Germany. He is a member of the Chemical Research on organic synthesis and catalysis relying on transition metal catalysis and visible photocatalysis.


FL-11

10-13 December 2023

Sustainable Synthetic Approaches to Spirocycles, Pentafulvenes and Spiropyrrolines from 1, 3-Indanediones

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2-(2'-keto alkyl)-1,3-serve as an important precursor for the construction of various bicyclic, spiro cyclic systems with suitable partners. Accordingly, the 2-keto-1,3-indandiones reaction of arynes with provided dibenzobicyclo[3.2.1]octadienone core¹ and the reaction of dimethyl acetylene dicarboxylate (DMAD) with 2/3-keto-1.3-Indandiones afforded spiro[4.4]nonane, spiro[4.5]decane compounds in presence of a catalytic amount of DABCO.² Moreover, the spiro[4.4]nonanes were transformed into highly conjugated pentafulvene motifs via unprecedented C-C bond rearrangement in an acidic medium. Similarly, we have also developed a catalyst-free method to access various 1,3-indandione-containing spiropyrrolines.



References

1. Hazra, G.; Mishra, G.; Dandela, R.; Thirupathi, B. J. Org. Chem. 2022, 87, 18, 11925-11938.

2. Mishra, G.; Sasmal, M.; Chakraborty, A. Thirupathi, B. Chem. Eur. J. 2023 (manuscript under revision).



10-13 December 2023

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Dr. Thirupathi Barla was born in Madavelli, Manchirial district, Telangana, India in 1984. After completing of M.Sc. (Organic Chemistry) from Osmania University (2006-2008), he worked as a research chemist at GVK-Biosciences, Hyderabad (2008-2009). In early 2009 he joined as a Junior Research Fellow (JRF) at CSIRIndian Institute of Chemical Technology, Hyderabad with Dr. D. K. Mohapatra for doctoral studies (2009-2014). Afterwards, he worked as an associate research scientist in-process R&D division at Sai Life Sciences, Hyderabad (2014-2015). Then Dr. Barla moved to Harvard University as a postdoctoral fellow to work with Prof. E. J. Corey (2015-2018) where he was involved in the development of highly active fluorinated secondgeneration oxazaborolidine catalysts and their application in Diels-Alder reactions. In July 2018, he became an Assistant Professor of Chemistry at the Indian Institute of Science Education and Research Berhampur. Dr. Thirupathi's area of research includes the total synthesis of biologically active natural products or model compounds having potential bioactivities. Dr. Thirupathi's group also works on the development of novel carbon-corban bond formation reaction and their application towards natural product synthesis.

Awards:

Thieme Chemistry Journal award-2023

Outstanding reviewer award from the journal, Tetrahedron Letters in August **2018**.

Postdoctoral fellowship from Harvard University, USA in 2015.



FL-12

10-13 December 2023

Unactivated Haloalkanes in C–C Bond Formation Reactions Veera Reddy Yatham*

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Alkyl radicals are powerful synthetic intermediates in organic chemistry for the construction of carbon–carbon and carbon-heteroatom bonds. In the early days, metal-based reagents (Sn, Mn, Si) were employed for the generation of alkyl radicals from alkyl C–X (X = Cl, Br, I) bonds through the halogen atom transfer (XAT) process.^[1] Recently, with the advent of photoredox catalysis a novel carbon-based abstractor, the α -aminoalkyl radical, became an ideal intermediate to perform XAT processes due to the simplicity of the methods to access it, the broadness and commercial availability of the tertiary amine precursors required, and the improved environmental footprint it.^[2] This lecture will be focussed on the generation of alkyl radicals from unactivated haloalkanes through XAT, single electron transfer (SET) and hydrogen atom transfer (HAT) followed by XAT and further applications in a variety of C-C bond formation reactions.^[3]



References

1. T. Constantin, F. Julia and D. Leonori, Chem. Rev. 2022, 122, 2292.

2. T. Constantin, M. Zanini, A. Regni, N. S. Sheikh, F. Juliá and D. Leonori, *Science* 2020, 367, 1021.

3. (a) G. S. Yedase, A. K. Jha and Veera Reddy Yatham *J. Org. Chem.* **2022**, *87*, 5442. (b) A. R. Tripathy, A. Kumar, R. A. Rizwana, A. K. Jha and V. R. Yatham, *Org. Lett.* **2022**, *24*, 5186. (c) A. R. Tripathy, R. A Rizwana, A. Kumar and V. R. Yatham, *Org. Biomol. Chem.* **2022**, *20*, *3136 - 314*. (d) A. R. Tripathy, A. Mishra, V. Singh, and V. R. Yatham, *Chem. Eur. J.* **2023**, *29*, e2023007.



10-13 December 2023

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Professional Experience:

August 2008 - Oct 2011

Assistant Professor, IISER-TVM, India.
Ramanujan fellow at CSIR-IICT, India.
Post. Doc, with Prof. Ruben Martin, Institute of Chemical Research of Catalonia (ICIQ), Spain.
Post. Doc, with Prof. Bukhard konig , University of Regensburg.
Ph.D. with Prof. Albrecht Berkessel, Universitof Cologne, Germany.

Master of Science (MS), IISc-Bangalore, India.



IL-35

10-13 December 2023

Responsible cosmetic ingredients: opening a new area of abundant minerals

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Since time immemorial, pigments from stones have been indispensable ingredients in cosmetics for makeup or sun protection. Minerals coming from the earth's crust are not renewable. Their feedstocks are more and more under the socio-economic lights and may cause strategic tensions. Sustainability in downstream industries using mineral resources has received growing interest from consumers who want industrials to take into account planetary boundaries and to preserve rare resources. Everybody has an opinion of what an abundant mineral is but when we want to explain and evaluate it, we face very complex questions. We perceive that we have to deal with geological data, but also environmental, technical, economic, social constraints. A methodology was lacking. That is why we have established the following strategy based on a multiparametric and rational approach involving the aggregation of a worldwide recognized set of data to define a new methodology for assessing non-energetic mineral resources abundance.

The first point is to define what an abundant mineral is. To answer this question, we have given this definition: abundant minerals refer to minerals which are naturally frequent on earth, easily accessible, essential for industrial usage and for which the quantity used to manufacture target products has only a tiny impact on the resource. And in order to give a quantitative aspect to this definition, we have completed it with the introduction of an abundant index which will be the key parameter to evaluate the criteria of abundance. A methodology (1) will be presented to calculate a Mineral Abundance Index (AI) applied to non-energy mineral resources (i.e. metals, industrial rocks and minerals). Based on a multi-criteria analysis, this index considers intrinsic natural mineral abundance (geosphere) and technical-economic mineral abundance (technosphere) while reconciling the stock-fixed and opportunity-cost paradigms by considering innovation (socio-epistemic sphere). The AI, graduated from 0 (very scarce) to 100 (very abundant) aims to qualify the abundance of minerals in a simple and rapid manner, based on published, reliable, supported and sourced data. Thus, the Mineral Abundance Index could be a powerful decision support tool for any downstream industry. This unique method shows the important efforts being made in the responsible cosmetic area to reduce environmental footprint and to fight against natural resources depletion.

References

1. N. Charles, R. Tuloup, A. Carreaud, F. Deswartes, V.Manzin, J. Aupoil, to be published.



10-13 December 2023

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Rémy Tuloup received his PhD in 1988 at the University Rennes I for work on dipolar reactions using diazomethane for the functionalization of cephems under the supervision of Pr. Robert Carrié and Pr. Danion. Then, he went to Cranfield University (United Kingdom) for a post-doctoral period where he studied biotechnologies, in particular the enzymatic synthesis of biopolymers within the group of Prof. Higgins. For more than 30 years at L'Oréal, he has used both conventional chemical routes for the synthesis of cosmetic ingredients (dyes, active compounds, tensors, etc.) and biotechnological ones. He is now in charge of evaluating the naturalness of ingredients, the abundance of minerals and the analysis of processes by making them comply with the rules of green chemistry.



IL-36

10-13 December 2023

Newly Developed Pd Catalysts for Challenging Csp²-Csp², Csp²-Csp³ and C-N Coupling for API Synthesis

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A new class of ferrocene-based unsymmetrical bis phosphines, $Fc(PAd_2)(PR_2)$ (R = Ph, Cy, iPr and tBu) named as MPhos ligands, their corresponding (MPhos)PdCl₂ complexes and *t*Bu₃P based oxidative addition complex, (*t*Bu₃P)Pd(*p*-CF₃C₆H₄)Br were developed for cross coupling applications. These complexes were effectively used as pre-catalysts for all types of Csp²-Csp³ coupling and CSp²-Csp² bond forming reactions involving challenging nucleophiles such as pentafluoro boron reagents. Applications were demonstrated for model and "drug-like" molecules to show the potential value of these catalysts in in API synthesis. The strategy behind the design of the catalysts and their applications in synthetic organic chemistry will be presented.

References

1. S. J. Firsan, V. Sivakumar, T. J. Colacot. *Chem. Rev.* 2022, **122 (23)**, 16983.

- 2. G. Xu, P. Gao, T. J. Colacot, ACS Catal. 2022, 12(9), 5123.
- 3. Y. N. Timsina, G. Xu, T. J. Colacot, ACS Catal. 2023, 13(12), 8106.

3. S. Hazra, C.C. C. Johansson Seechurn, S. Handa, and T. J. Colacot, ACS Catal. 2021, **11(21)**, 13188.

4. P. M. MacQueen, R. Holley, S. Ghorai, T. J. Colacot, Organometallics 2023, ASAP

5. *New Trends in Cross-Coupling: Theory and Applications*; T. J. Colacot, Ed.; RSC: Cambridge, 2015; ISBN: 978-1-84973-896-5A.

6. C. C. C. Johansson-Seechurn, M. O. Kitching, T. J. Colacot, V. Snieckus, Angew Chem. 2012, **51(21)**, 5015.



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Thomas J. Colacot joined MilliporeSigma (a business of Merck KGaA, Darmstadt, Germany) in 2018 as an R&D Fellow and Director of Global Technology Innovation, Life Science Business, in Milwaukee, WI. He has extensive experience in developing new and innovative products and technology with a very strong track record of commercialization globally and is considered an industrial expert in organometallics and homogeneous catalysis for organic synthesis. He has over 120 peer-reviewed publications, three books and about 70 patents internationally. Thomas is a recipient of many awards and honors, including the 2021 Scientific Curriculum Vitae (Life Time Achievement Award) from the Chairman of the Board and CEO of Merck KGaA, Darmstadt, Germany; the 2018 Outstanding Researcher Award from Merck KGaA, Darmstadt, Germany; the 2017 Catalysis Club of Philadelphia Award for outstanding contributions in the area of catalysis; the 2015 ACS Industrial Chemistry Award; the 2015 IPMI Henry Alfred Award; the 2016 Indian Institute of Technology Madras Distinguished Alumnus Award for Technology Innovation; the 2016 Chemical Research Society of India (CRSI) Medal; and the 2012 RSC Applied Catalysis Award and Medal. Dr. Colacot was responsible for developing a very successful homogeneous catalysis program at Johnson Matthey from 1995 to 2018. He holds an MBA degree from Penn State University and a Ph.D. degree in chemistry from IIT Madras. He has also carried out postdoctoral work in the U.S. and is a fellow of the Royal Society of Chemistry. He has given more than 400 presentations globally. He is a visiting professor of IIT Bomaby Mumbai, VIT Vellore, IISER Thiruvanathapuram and IIRBS, MG University.