International Conference on Organometallics and Catalysis 2020

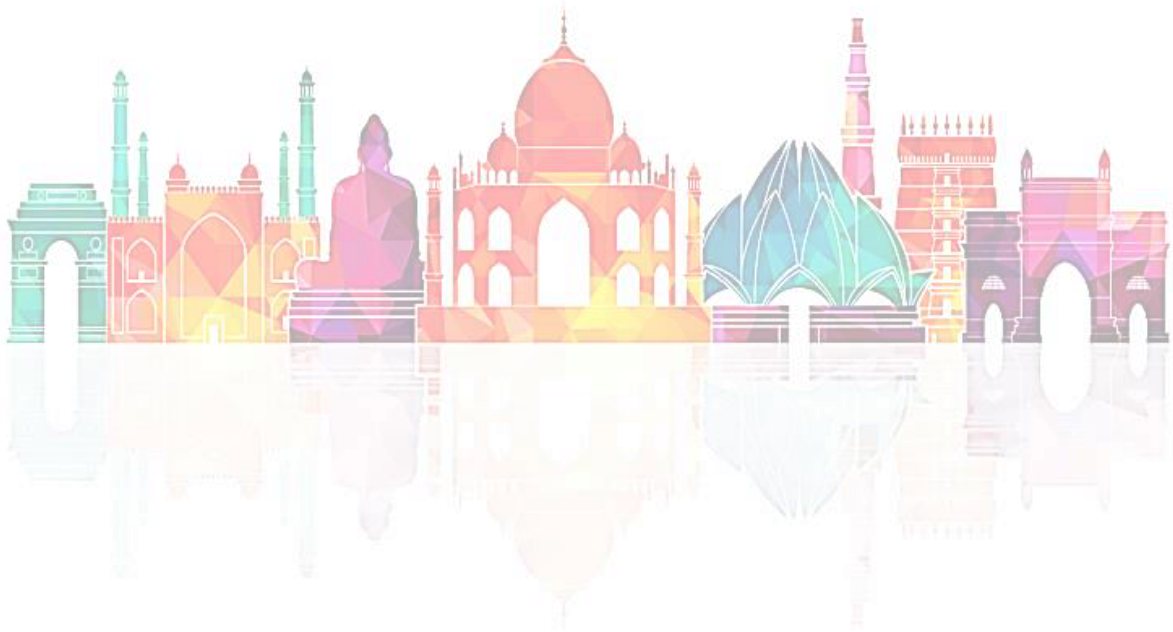
Programme and Abstracts

March 7-10, 2020

Holiday Inn Resort, Goa

ABOUT ICOC 2020 CONFERENCE

This international conference is expected to intensify scientific interaction among leading researchers around the world from both industry and academia. It will enable the researchers to identify possible areas where collaborative work may be useful for better understanding of a complex system or designing new catalysts and materials.



Scientific programme will include the broad spectrum of Inorganic and Organic Chemistry covering Organometallics and Catalysis, Photocatalysis, Organocatalysis, Coordination Chemistry, Bio-inorganic chemistry, Asymmetric catalysis, Supramolecular Chemistry and computational chemistry. The conference will include oral and poster presentations.

ABOUT THE VENUE

The Conference will take place at 'Holiday Inn Resort', located on the picturesque Mobor beach in South Goa. 'Holiday Inn Resort' is 51 Km away from the Goa International Airport (Dabolim Airport).
Goa is a small state situated on the western coast of India. It was liberated from the rule of Portuguese in 1961 and is the 25th State of India. Located on the Western Ghats of Konkan, Goa is known as the smallest and the fourth smallest populated state in India. Goa is bounded by Maharashtra to its north, eastern and southern boundaries were formed by Karnataka, while the western coast is formed by the Arabian Sea.

International and domestic tourists visit this tiny state every year, in a large number. Tourists are attracted to its golden beaches, architecture and places of worship. It is a biodiversity hotspot and is rich in flora and fauna. Goa is known for sharing harmonious relationship among its various religious communities, living peacefully for generations.

PLACE AND CLIMATE

The best time to visit Goa is during the winters. This time of the year offers a pleasant weather in Goa and draws in tourists and festivities. It is ideal to plan a perfect family holidays and even if you are with your friends the season is surely not going to bore you. The minimum temperature goes down to 15°C and the maximum temperature in Goa in November to January roves between 20°C to 25°C.

PLACES TO VISIT

Tourist visit the following places in Goa

Panaji, Calangute Beach, Baga Beach, Anjuna Beach, Dona Paula, Colva Beach, Palolem Beach, Fort Aguada, Morjim Beach, Dudhhsagar Waterfalls

ORGANIZING TEAM

Organizing Committee

Prof. Swadhin Mandal, IISER Kolkata

Prof. Debabrata Maiti, IIT Bombay

Prof. Akkattu T. Biju, IISc Bangalore

Prof. Santanu Mukherjee, IISc Bangalore

Prof. Alakesh Bisai, IISER Bhopal

Prof. Modhu Sudan Maji, IIT Kharagpur

Prof. Basker Sundararaju, IIT Kanpur

Prof. Sundargopal Ghosh, IIT Madras

Prof. Partha Sarathi Mukherjee, IISc Bangalore

Prof. Pierre Dixneuf, Institut des Sciences Chimiques de Rennes, France

Prof. Uttam Tambar, University of Texas Southwestern Medical Center, USA

Prof. Daniel B. Werz, Technische Universität Braunschweig, Germany

Dr. Subhendu Kumar Mohanty, Syngene International Limited, Bangalore

Dr. Abhisek Dutta Chowdhury, Wuhan University, China

Dr. Chandra Kanta De, Max-Planck-Institut für Kohlenforschung, Germany

Dr. Deeksha Gupta, Managing Editor, ACS Publications

Dr. Aparna Ganguly, Editorial Development Manager at Royal Society of Chemistry

Prof. Nidhi Jain, Associate Professor, IIT Delhi

Dr. Dinesh Talwar, Associate Editor, Wiley-VCH

Dr. Dietmar Hueglin, BASF Chemicals India Pvt Ltd

Prof. Biprajit Sarkar, Freie Universität Berlin

Prof. Stellios Arseniyadis, Queen Mary University of London

Dr. Rakeshwar Bandichhor, Director and CoE-Chemistry Head-API-R&D, ACS-India Chapter

International Conference on Organometallics and Catalysis (ICOC 2020)

Biosketch of Swadhin K Mandal

Dr. Swadhin K Mandal, FRSC
Professor and Head

Department of Chemical Sciences
Indian Institute of Sciences Education and Research Kolkata
Address: Mohanpur-741246

E-mail: swadhin.mandal@iiserkol.ac.in

Nationality: Indian

Academic and Professional Career

Current Position: Professor (since 2018 October), Department of Chemical Sciences, IISER Kolkata and Associate Professor (2013 Dec.– till date): Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata

Assistant Professor (2007 July-2012 December): Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata

Alexander von Humboldt Postdoctoral Fellow (2006-2007) with Prof Herbert W Roesky: University of Goettingen, Germany.

Postdoctoral Fellow (2002- 2006) with Prof. Robert C Haddon: University of California, Riverside, USA.

Ph.D. (1996-2002): Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India. Supervisor: Prof. S S Krishnamurthy

M.Sc. (Chemistry, 1994-1996): University of Kalyani, Kalyani, India. (Secured 1st rank in the University)

B.Sc. (Chemistry, 1990-1994): University of Kalyani, Kalyani, India. (Secured 3rd rank in the University)

Awards and Professional Recognition:

♦ *Shanti Swarup Bhatnagar Prize in Chemical Sciences for 2018*

♦ Invited as *Editorial Advisory Board member* of the journal 'Inorganic Chemistry' published by the American Chemical Society during 2019-2022

♦ Fellow of Royal Society of Chemistry (FRSC) under the "Leaders in the Field" category.

♦ Awarded with SERB Distinguished Investigator Award.

♦ CRSI bronze medal, 2019

♦ Editorial advisory board member *J. Chem Sci.* since 2018

♦ *YIM-Young Scientist Award -2012* by YIM-Boston held during 6-8th October, 2012 at MIT, Boston, USA.

♦ Served as *Editorial Advisory Board member* of the journal 'Organometallics' published by the American Chemical Society during 2013-2015

♦ Alexander von Humboldt fellowship (2006).

Bio-Sketch of Debabrata Maiti

Dr. Debabrata Maiti
Associate Professor

Department of Chemistry
IIT Bombay
Powai, Mumbai 400 076, Maharashtra, INDIA

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Homepage: https://www.dmaiti.com/

Education:

- **Ph. D.,** Department of Chemistry, Johns Hopkins University, USA (2003-2008)
  (Supervisor: Prof. Kenneth D. Karlin)
- **M. Sc.** IIT Bombay, India (2001-2003)
- **Postdoctoral study**: Massachusetts Institute of Technology, USA (2008-2010)
  (Supervisor: Prof. Stephen L. Buchwald)

Research and Teaching Experience:

- Assistant Professor, IIT Bombay, Department of Chemistry, India (2010-2015)
- Associate Professor, IIT Bombay, Department of Chemistry, India (2015-present)

Selected Awards, Honours, Recognitions:

- Humboldt Research Fellowship for Experienced Researchers 2020
- FRSC, Fellow of the Royal Society of Chemistry 2019
- NASI Scopus Young Scientists Award- Innovation in Engineering and Physical Sciences 2019

Research interests:

Site selective remote C–H functionalization for both aliphatic and arene systems, Photoredox catalysis, Bioinspired catalysis.

Membership of professional societies:

Associate Editor, The Journal of Organic Chemistry,
Editorial Board member of Chemistry - A European Journal,
Editorial Advisory Board, Organometallics
International Advisory Board of Chemistry - An Asian Journal,
Early Career Board Member, Inorganica Chimica Acta,
Visiting Faculty, WRHI, Tokyo Institute of Technology, Japan,
Visiting Faculty, University of Pavia, Italy.

Bio-Sketch of A. T. Biju

Dr. A. T. Biju
Associate Professor

Editor-in-Chief, *J. Heterocyclic Chem*. (Wiley)

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A. T. Biju received his M. Sc. from Sacred Heart College Thevara (affiliated to MG University, Kerala, India) and Ph.D. under the guidance of Dr. Vijay Nair at the CSIR-NIIST (Formerly RRL), Trivandrum, India. Subsequently, he has been a post-doctoral fellow with Prof. Tien-Yau Luh at the National Taiwan University, Taipei and an Alexander von Humboldt fellow with Prof. Frank Glorius at the Westfälische Wilhelms-Universität Münster, Germany. In June 2011, he began his independent research career at the CSIR-National Chemical Laboratory, Pune. From June 2017 onwards, he has been an Associate Professor at the Department of Organic Chemistry, Indian Institute of Science, Bangalore. His research focuses on the development of transition-metal-free carbon-carbon and carbon-heteroatom bond-forming reactions using aryne chemistry and N-heterocyclic carbene (NHC) organocatalysis, and their application in organic synthesis.

Program Schedule

International Conference on Organometallics and Catalysis 2020

Holiday Inn Resort, Goa (Mar. 7-10, 2020)

7th Mar., 2020 (Saturday)		
13.30-14.40	Registration	
14:40 - 14:45	Welcome remarks by Prof. Swadhin Mandal, IISER Kolkata & Prof. A. T. Biju, IISc Bangalore	
Session 1 Chairperson: Prof. Matthias Driess, TU Berlin		
IL-01 (14:45-15:15)	Prof. Christopher W. Jones, Georgia Tech	
IL-02 (15:15-15:45)	Prof. Franc Meyer, University of Göttingen	
IL-03 (15:45-16:15)	Prof. F. Dean Toste, University of California, Berkeley	
IL-04 (16:15-16:45)	Prof. David Lupton, Monash University	
IL-05 (16:45-17:15)	Prof. P. H. Dixneuf, Université de Rennes	
Tea/Coffee Break (17:15-17:35)		
Session 2 (Parallel Session) Chairperson: Prof Mark Lautens University of Toronto		**Session 3 (Parallel Session)** Chairperson: Prof. Jennifer Love, University of British Columbia
IL-06 & 07 (17:35-17:55)	IL-06: Prof. Rajarshi Samanta IIT Kharagpur	IL-07: Prof. Dibyendu Das IISER Kolkata
IL-08 & 09 (17:55-18:15)	IL-08: Prof. Joyram Guin IACS Kolkata	IL-09: Prof. Arnab Rit IIT Madras
IL-10 & 11 (18:15-18:35)	IL-10: Prof. Rafal Kowalczyk Polish Academy of Sciences	IL-11: Prof. Dmitry Katayev ETH Zurich
IL-12 & 13 (18:35-18:55)	IL-12: Prof. S. Katukojvala IISER Bhopal	IL 13: Prof. Ajay Venugopal IISER TVM
IL-14 & 15 (18:55-19:15)	IL-14: Prof. Mahiuddin Baidya IIT Madras	IL-15: Prof. Prasanta Ghosh RKM residential College
IL-16 & 17 (19:15-19:35)	IL-16: Prof. R Vijaya Anand IISER, Mohali	IL-17: Prof. Anukul Jana TIFR Hyderabad
19:35 onwards	**Dinner & Networking**	
8th Mar., 2020 (Sunday)		
Session 4 Chairperson: Prof. H. Ila, JNCASR, Bangalore		

IL-18 (09:00-09:30)	Prof. Huw M. L. Davies, Emory University
IL-19 (09:30-10:00)	Prof. Marisa Kozlowski, University of Pennsylvania
IL-20 (10:00-10:30)	Prof. Jitendra K. Bera, IIT Kanpur
Tea/Coffee Break (10:30-11:00)	
Session 5 (RSC) Chairperson: Dr Aparna Ganguly, RSC India	
IL-21 (11:00-11:30)	*Chem. Commun*. Lecture: Prof. Douglas W. Stephan University of Toronto
IL-22 (11:30-12:00)	*Dalton Trans.* & *Catal. Sci. Technol.* Lecture Prof. Jennifer Love, University of British Columbia
IL-23 (12:00-12:30)	Prof. Mark Lautens, University of Toronto
IL-24 (12:30-13:00)	Prof. Sayam Sengupta IISER Kolkata
Lunch Break (13:00 - 14:00)	

Session 6 (Parallel Session) Chairperson: Dr. Dinesh Talwar Wiley Publishing		**Session 7 (Parallel Session)** Chairperson: Dr. Ajay Jha, ACS Publishing
IL-25 & 26 (14:00-14:20)	IL-25: Prof. Alakananda Hajra Viswa-Bharati University	IL-26: Prof. Tarun Kanti Panda IIT Hyderabad
IL-27 & 28 (14:20-14:40)	IL-27: Prof. R. G. Bhat IISER Pune	IL-28: Prof. Vandana Bhalla GNDU Amritsar
IL-29 & 30 (14:40-15:00)	IL-29: Prof. Chandan K. Jana IIT Guwahati	IL-30: Prof. Pierre Kennepohl University of British Columbia
IL-31 & 32 (15:00-15:20)	IL-31: Prof. Amit Kumar IIT Patna	IL-32: Prof. Shabana Khan IISER Pune
IL-33 & 34 (15:20-15:40)	IL-33: Prof. Suman De Sarkar IISER Kolkata	IL-34: Prof. Sakya Sen CSIR-NCL, Pune
IL-35 & 36 (15:40-16:00)	IL-35: Prof. Pradip Maity CSIR-NCL Pune	IL-36: Prof. Arnab Datta IIT Gandhinagar

Tea/Coffee Break (16:00-16:20)	
16:20 to 18:20 Flash Talks (~20 Nos), then Poster Session Chairperson: Prof. Basker Sundararaju, IIT Kanpur	
19:30 onwards	**Conference Dinner & Networking**
9th Mar., 2020 (Monday)	
Session 8 Chairperson: Prof. Sourav Pal, Director, IISER Kolkata	

IL-37 (08:30-09:00)	Prof. William Tolman, Washington University in St. Louis
IL-38 (09:00-09:30)	Prof. Milton “Mitch” R. Smith, Michigan State University
IL-39 (09:30-10:00)	Prof. Frank Glorius, University of Münster
IL-40 (10:00-10:30)	Prof. Michael Greaney, University of Manchester

Tea/Coffee Break (10:30-11:00)

Session 12
Chairperson: Prof. Goutam K. Lahiri, IIT Bombay

IL-41 (11:00-11:30)	Prof. Holger Braunschweig, University of Würzburg
IL-42 (11:30-12:00)	Prof. Dr. Matthias Tamm, TU Braunschweig
IL-43 (12:00-12:30)	Prof. Dr. F. Ekkehardt Hahn, University of Münster
IL-44 (12:30-13:00)	Prof. Tapan Kanti Paine, IACS Kolkata

Lunch Break (13:00 - 14:00)

	Session 13 (Parallel Session) Chairperson: Prof. Santanu Mukherjee, IISc Bangalore	**Session 14 (Parallel Session)** Chairperson: Prof. Partha Sarathi Mukherjee, IISc Bangalore
IL-45 & 46 (14:00-14:30)	IL-45: Prof. Daniel Werz TU Braunschweig	IL-46: Prof. Sundargopal Ghosh IIT Madras
IL-47 & 48 (14:30-15:00)	IL-47: Prof. C. V. Ramana CSIR-NCL Pune	IL-48: Prof. Kumar Vanka CSIR-NCL Pune
IL-49 & 50 (15:00-15:30)	IL-49: Prof. Nitin Patil IISER Bhopal	IL-50: Prof. Biprajit Sarkar Frie University, Berlin
IL-51 & 52 (15:30-16:00)	IL-51: Prof. Stellios Arseniyadis Queens Mary Uty of London	IL-52: Prof. Zoltán Novák Eötvös Loránd University

Tea/Coffee Break (16:00-16:30)

16:30 to 18:30 Flash Talks (~20 Nos), then Poster Session
Chairperson: Prof. Basker Sundararaju, IIT Kanpur

19:30 onwards **Dinner & Networking**

10th Mar., 2020 (Tuesday)

Session 16
Chairperson: Prof. Frank Glorius, University of Münster

IL-53 (09:00-09:30)	Prof. Thomas R. Ward, University of Basel
IL-54 (09:30-10:00)	Prof. Bernhard Breit, University of Freiburg
IL-55 (10:00-10:30)	Prof. Lukas J. Gooßen, Ruhr-Universität Bochum

Tea/Coffee Break (10:30-11:00)	
Session 17 Chairperson: Prof. Jitendra Bera, IIT Kanpur	
IL-56 (11:00-11:30)	Prof. Matthias Driess, TU Berlin
IL-57 (11:30-12:00)	Prof. Motomu Kanai, University of Tokyo
Concluding Remarks	
(12:00-12:10)	Prof. Sourav Pal, Director, IISER Kolkata
(12:10-12:20)	Vote of Thanks Prof. Debabrata Maiti, IIT Bombay
Lunch & Departure (12:20 - 14:00)	

PARTICIPANTS

Participant

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch

Dr. Bryden Le Bailly

Designation Senior Editor, *Nature*

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Bryden Le Bailly is a Senior Editor at *Nature*. He joined the journal in November 2016 as the editor responsible for handling scientific research at the interface of chemistry and biology, after working at *Nature Nanotechnology* as a locum editor. As well as being responsible for publishing high-impact research, Bryden works closely with his journalistic and editorial colleagues in disseminating the implications of these studies to the broader scientific community. Prior to becoming an editor, he spent several years in chemical research, completing his PhD at the University of Manchester in 2016, followed by a post-doctoral/lab manager position at the University of Bristol. First working on iron catalysis, Bryden then investigated signal transduction through cell membranes using synthetic receptors, for which he received a STEM for Britain award from members of the Houses of Parliament.

INVITED LECTURES

Flow Reactors May Enable Efficient Rhodium-Catalyzed C-H Activation in Organic Synthesis

Chunjae Yoo,[a] Eric G. Moschetta,[a] Kathryn M. Chepiga,[b] Daniel Rackl,[b] Solymar Negretti,[b] Nicholas A. Brunelli,[a] Ryan P. Lively, [a] Huw M. L. Davies[b] and Christopher W. Jones[a]*

[a]*School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA*

[b]*Department of Chemistry, Emory University, Atlanta, GA 30322, USA*

**Corresponding author: cjones@chbe.gatech.edu*

Abstract:

C–H functionalization is an emerging synthetic strategy allowing for innovation in total synthesis and new methodologies for drug development. One particularly useful C–H functionalization procedure has been the C–H insertion chemistry of transient metal carbenes, which are typically generated from diazo compounds.(1) As an example, rhodium-stabilized donor/acceptor carbenes have been shown to be highly effective in a wide range of intermolecular C–H functionalization reactions, in which the site selectivity and stereoselectivity are dominated by catalyst control.(2) However, a potential drawback of the use of diazo compounds as carbene precursors is the issue of safe handling of large quantities of these high-energy compounds. Additionally, Rh catalysts can be quite expensive, and methodologies of maximizing catalyst turnover number and potentially recovering Rh for reprocessing are needed.

Three advances will be described in this lecture, all developed in the Center for C-H Functionalization (CCHF). First, a new type of microfluidic flow reactor was developed based on polymeric hollow fibers that have been deployed large scale gas separations.(3). Second, modified Rh_2 complexes that are can be grafted onto solid supports have been developed.(4,5) Third, the utilization of the Rh catalysts in several enantioselective coupling reactions has been demonstrated in flow, including in conjunction with on-demand, flow synthesis of the reactive diazonium compounds.(5,6)

References

1. H. M. L.,Davies, D. Morton, *Chem. Soc. Rev*. **40**, 1857-1869 (2011)
2. K. Liao, S. Negretti, D. G. Musaev, J. Bacsa, H. M. L. Davies, *Nature* **533**, 230-234 (2016).
3. E. G. Moschetta, S. Negretti, K. M. Chepiga, N. A. Brunelli, Y. Labreche, Y. Feng, Fateme Rezaei, R. P. Lively, W. J. Koros, H. M. L. Davies, C. W. Jones, *Angew. Chem. Int. Ed*. **54**, 6570-6574 (2015).
4. K. M. Chepiga, Y. Feng, N. A. Brunelli, C. W. Jones, H. M. L. Davies, *Org. Lett*. **15**, 6136-6139, (2013)
5. D. Rackl, C.-J. Yoo, C. W. Jones, H. M. L. Davies, *Org. Lett*. **19**, 3055-3058, (2017)
6. C.-J. Yoo, D. Rackl W. Liu C. B. Hoyt B. Pimentel, M. L. Davies, C. W. Jones, *Angew. Chem. Int. Ed*. **57**, 10923-10927 (2018).

Invited Lecture (IL-01)

International Conference on Organometallics and Catalysis (ICOC 2020)

Biosketch of Speaker

Dr. Christopher W. Jones
Professor & William R. McLain Chair

School of Chemical & Biomolecular Engineering
Georgia Institute of Technology

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Chris Jones was born in suburban Detroit, Michigan in July of 1973. After his primary and secondary schooling 14 years in Troy, Michigan, he enrolled as a chemical engineering student at the University of Michigan. In route to earning a BSE in chemical engineering, Chris carried out research on transition metal carbide and nitride catalytic materials under the direction of Levi Thompson. After graduating in 1995, Chris moved to Pasadena, California, to study inorganic materials chemistry and catalysis under Mark E. Davis at Caltech. There he earned MS and PhD degrees in chemical engineering in 1997 and 1999, respectively. Subsequently, he studied organometallic chemistry and olefin polymerization under the direction of both Davis and John E Bercaw at Caltech. He started as an Assistant Professor at Georgia Tech in the summer of 2000 and was promoted to Associate Professor in July 2005. In May, 2005, he was appointed the J. Carl and Sheila Pirkle Faculty Fellow, followed by a promotion to Professor in July 2008. He was named New-Vision Professor of Chemical & Biomolecular Engineering in July 2011. In 2015, he became the Love Family Professor of Chemical & Biomolecular Engineering, and in 2019 the William R. McLain Chair. Chris was named the Associate Vice President for Research at Georgia Tech in November 2013. In this role, he directed 50% of his time on campus-wide research administration with a primary focus on interdisciplinary research efforts and policy related to research institutes, centers and research core facilities. In 2018, he served as the Interim Executive Vice-President for Research, before returning full time to his research and teaching roles in chemical and biomolecular engineering in 2019.

Dr. Jones directs a research program focused primarily on catalysis and CO_2 separation, sequestration and utilization. In 2010 he was honored with the *Ipatieff Prize* from the American Chemical Society for his work on palladium catalyzed Heck and Suzuki coupling reactions. That same year, he was selected as the founding Editor-in-Chief of *ACS Catalysis*, a new multi-disciplinary catalysis journal published by the American Chemical Society. In 2013, Chris was recognized by the North American Catalysis Society with the *Paul E. Emmett Award in Fundamental Catalysis* and by the American Society of Engineering Education with the *Curtis W. McGraw Research Award*. Most recently, he was recognized by the American Institute of Chemical Engineers with the 2016 *Andreas Acrivos Award for Professional Progress in Chemical Engineering*, distinguishing him as one of the top academic chemical engineers under 45. Dr. Jones has been PI or co-PI on over $63M in sponsored research in the last sixteen years, and as of July 2019, has published over 280 papers that have been cited >21,000 times. He has an H-Index of 75 (Google Scholar).

Invited Lecture (IL-02)
International Conference on Organometallics and Catalysis (ICOC 2020)

Bioinspired Small Molecule Activation for Energy-Related Catalysis

Franc Meyer*
Institute of Inorganic Chemistry
Georg-August-University Göttingen, Germany
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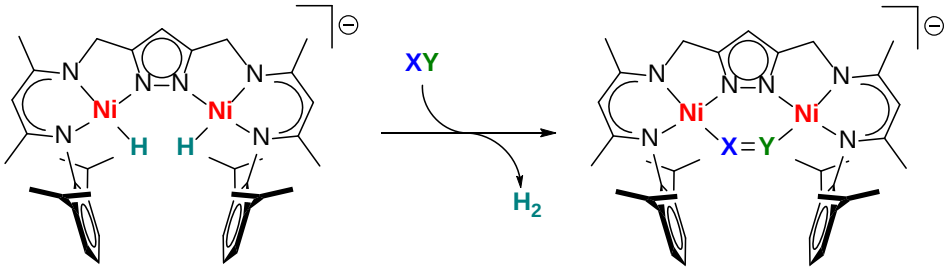
Abstract:
Understanding the functional principles of metalloenzymes offers great inspiration for the development of novel bioinspired catalysts, most importantly for catalysts relevant to the global energy challenge. For achieving the activation and transformation of small molecules, enzymes often take advantage of the cooperative action of two or more proximate metal ions hosted within the protein active site. Work in our group has exploited the use of compartmental pyrazolate-based ligand scaffolds for hosting two metal ions at tuneable distances to enable beneficial metal-metal cooperativity, and to emulate bioinorganic reactivity and isolate key intermediates.[1]
Recently we have developed highly preorganized dinuclear nickel hydride complexes that can reductively bind challenging substrates concomitant with the release of H_2 (Figure 1),[2-5] which is akin to the N_2 activation step in biological nitrogenase. These new systems and their use for the bioinspired activation and transformation of small molecules such as O_2, H_2, NO, N_2, etc. will be discussed in the lecture.

Figure 1:



References:

1. (a) Klingele, J.; Dechert, S.; Meyer, F. *Coord. Chem. Rev.* **2009**, *253*, 2698-2741; (b) Dalle, K. E.; Meyer, F. *Eur. J. Inorg. Chem.* **2015**, 3391-3405.
2. Manz, D.-H.; Duan, P.-C.; Dechert, S.; Demeshko, S.; Oswald, R.; John, M.; Mata, R. A.; Meyer, F. *J. Am. Chem. Soc.* **2017**, *139*, 16720-16731.
3. Duan, P.-C.; Manz, D.-H.; Dechert, S.; Demeshko, S.; Meyer, F. *J. Am. Chem. Soc.* **2018**, *140*, 4929-4939.
4. Ferretti, E.; Dechert, S.; Demeshko, S.; Holthausen, M. C.; Meyer, F. *Angew. Chem. Int. Ed.* **2019**, *58*, 1705-1709.
5. Ferretti, E.; Dechert, S.; Meyer, F. *Inorg. Chem.* **2019**, *58*, 5154-5162.

Invited Lecture (IL-02)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

Dr. Franc Meyer
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Franc Meyer (born in 1965) earned his Ph.D. in the field of synthetic azaborane cluster chemistry with Peter Paetzold at RWTH Aachen in 1993. He continued his studies as a postdoctoral researcher with Peter Armentrout at the University of Utah where he used gas phase guided ion beam methods to determine metal-ligand bond dissociation energies. On returning to Germany, he completed his habilitation under the mentorship of Gottfried Huttner at Ruprecht Karls University Heidelberg in 2000 and became Professor of Inorganic and Bioinorganic Chemistry at Georg-August-University Göttingen in 2001. He is a member of the Göttingen Academy of Sciences, the Royal Physiographic Society in Lund/Sweden, and the German National Academy of Sciences Leopoldina. He served on various panels of the German Research Foundation (DFG) including the DFG Senate, he is a member of the Research Advisory Board of the Fonds der Chemischen Industrie (FCI) and he is vice chair of the Wöhler Association for Inorganic Chemistry of the German Chemical Society (GDCh). Since 2013 he is an Associate Editor of the ACS journal *Inorganic Chemistry*. His research focuses on the activation of small molecules and on cooperative effects in bimetallic and multimetallic complexes, with particular interests in bioinorganic chemistry, bioinspired catalysis and magnetic nanoswitches.

Selectivity as Inspiration for Catalysis

F. Dean Toste*
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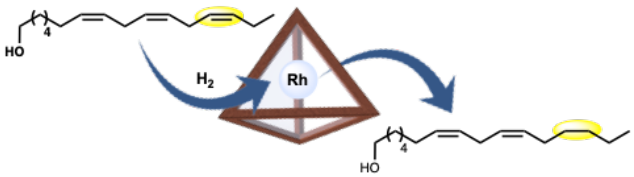
Abstract:
Selective reactions are a cornerstone of modern organic synthesis, enabling sustainable access to fine chemicals and pharmaceuticals. This lecture will focus on the development of organic reactions and reagents that allow for selective reaction ranging from enantioselective transformations to chemoselective modifications of complex structures. Strategies leveraging homogeneous transition metal catalysis,[1] chiral anion catalysis[2] and supramolecular catalysis[3] to achieve these selectivities will be discussed.



References and Notes:

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Invited Lecture (IL-03)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Gerald E. K. Branch Distinguished Professor

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Education

Ph.D. Chemistry, Stanford University, Stanford, CA (2000)
M.Sc. Chemistry, University of Toronto, Toronto, ON, Canada (1995)
B.Sc. Chemistry and Biochemistry, University of Toronto, Toronto, ON, Canada (1993)

Academic Career

Gerald E. K. Branch Distinguished Professor, UC Berkeley (2017-present)
Professor, Department of Chemistry, UC Berkeley (2009-2017)
Faculty Scientist, Chemical Sciences Division, LBNL (2007-present)
Associate Professor, Department of Chemistry, UC Berkeley (2006-2009)
Assistant Professor, Department of Chemistry, UC Berkeley (2002-2006)
Postdoctoral Research Associate, Caltech (2001-2002)

Selected Awards and Recognitions

Elected Fellow of the American Academy of Arts and Science (2018); RSC, Catalysis in Organic Chemistry Award (2018); Janssen Prize (2018); Humboldt Research Award (2016); Elected Fellow of the Royal Society of Canada – Academy of Science (2015); GDCh Horst-Parcejus Preis (2015); ACS Creativity in Synthetic Organic Chemistry Award (2015); Mitsui Catalysis Award (2014); Mukaiyama Award (2011); Tetrahedron Young Investigator Award (2011); RSC Merck Award (2010); Thieme-IUPAC Prize in Synthetic Organic Chemistry (2008); ACS Elias J. Corey Award (2008); BASF Catalysis Award (2007); OMCOS Award (2007); ACS, Cope Scholar Award (2006); Alfred P. Sloan Fellow (2005); NSF CAREER Award (2005); Research Innovation Award (2002); Camille and Henry Dreyfus New Faculty Award (2002); ACS Nobel Laureate Signature Award (2002).

NHC-organocatalysis exploiting unusual reactive intermediates

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Abstract:
In 1962 Price observed the formation of homoenolate intermediates when acrylonitrile is exposed to phosphine catalysts in the presence of alcohols.[1] More recently, studies from our group, and others, have focused on reaction discovery through related species formed under NHC catalysis.[2] In this presentation I will focus on our recent studies with this intermediate and related structures that have enabled discoveries in synthesis.[3,4] This family of intermediates is extremely robust and can be deployed in a range of polar[3] and none polar reaction designs.[4]

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Invited Lecture (IL-04)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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David was born in South Australia, and received his undergraduate education at the University of Adelaide graduating with a BSc (Honours, 1st class) in 2001. In 2005 he completed his PhD studies at the Australian National University, supervised by Professor Martin G. Banwell. Between 2005 and 2007, Dr Lupton was a postdoctoral fellow with Professor Barry M. Trost (Stanford University) supported by the American Australian Association (Sir Keith Murdoch fellow). In 2007, he commenced an academic appointment at Monash University, receiving an Australian Research Council Future Fellowship in 2011 and promotion to Full Professor in 2018. His group is focused on the use of enantioselective catalysis to uncover novel reactivity and enable chemical synthesis.

Invited Lecture (IL-05)
International Conference on Organometallics and Catalysis (ICOC 2020)

Fast Functionalization of Pyridines and Phosphines with Ru(II) and Rh(I) catalysts

Pierre H. Dixneuf* Chang Sheng Wang Zhuan Zhang and Jean François Soulé
Institut Sciences Chimiques de Rennes, UMR 6226
University of Rennes-CNRS, RENNES, France
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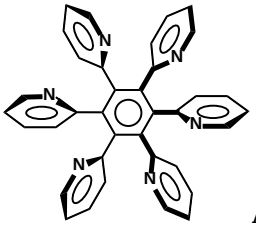
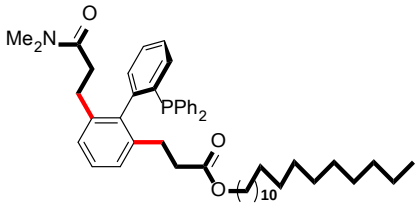
Abstract:
Ruthenium(II) catalysts associated to a carboxylate partner are able to promote the selective directed sp^2 C-H bond activation/deprotonation of functional arenes [1] even in water without surfactant. [2]. The lecture will present several new aspects based on these activation principles.
- **Ruthenium(II)-catalyzed** sp^2 C-H bond activation/functionalization in water can be directed to produce Hexaheteroarylbenzenes and hexadentate ligands of type **A**[3] and thus they offer new Ru, Pd, Pt catalysts.

-Ruthenium-catalyzed alkylations of ortho C-H bonds of phosphine oxides with alkenes can give access to new bifunctional phosphines. [4].



A



B

-Rhodium(I) catalysts by contrast can regioselectively functionalize the C-H bond of biaryl group of phosphines at ortho' position via formal insertion of alkene to produce functional dialkylated phosphines of type **B .** .[5]

It will be shown that these ligands can be used for efficient carboxylation of arylbromides with CO_2 with the help of a photocatalyst.

These green catalytic processes offer new routes for the building of polyfunctional ligands which have potential for the creation of efficient catalysts and for the design of new photoredox systems. [6]

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Invited Lecture (IL-05)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Pierre H. Dixneuf has initially worked on Ferrocene Chemistry and on N-Heterocyclic Carbene NHC metal complexes. After experiences in metal complex chemistry he started homogeneous catalysis at the University of Rennesin 1985 first with Ruthenium catalysts.
He developed first selective activation of alkynes and incorporation of CO_2, such as vinylcarbamates, via ruthenium-vinylidenes, -allenylidenes, and alkene metathesis catalysts and transformations of plant oils.
He is now contributing to C–H bond activation/functionalization using ruthenium(II) catalysts especially operating in water. As Emeritus professor he currently develops fast modifications of Phosphine and Pyridine derivatives.
He has co-authored more than 460 publications, co-edited 7 books and his work has been acknowledged with several prizes including: A. v Humboldt prize for Research 1990, Grignard-Wittig Prize (GDCh) 2000, Institut universitaire de France 2000, académie des sciences IFP prize, Sacconi medal (Italy) in 2006 and Chinese Society of Chemistry awards in 2014.

Step-Economic Syntheses of Nitrogen-Containing Extended π-Conjugated Systems via Metal-Carbene/Nitrene Migratory Insertions

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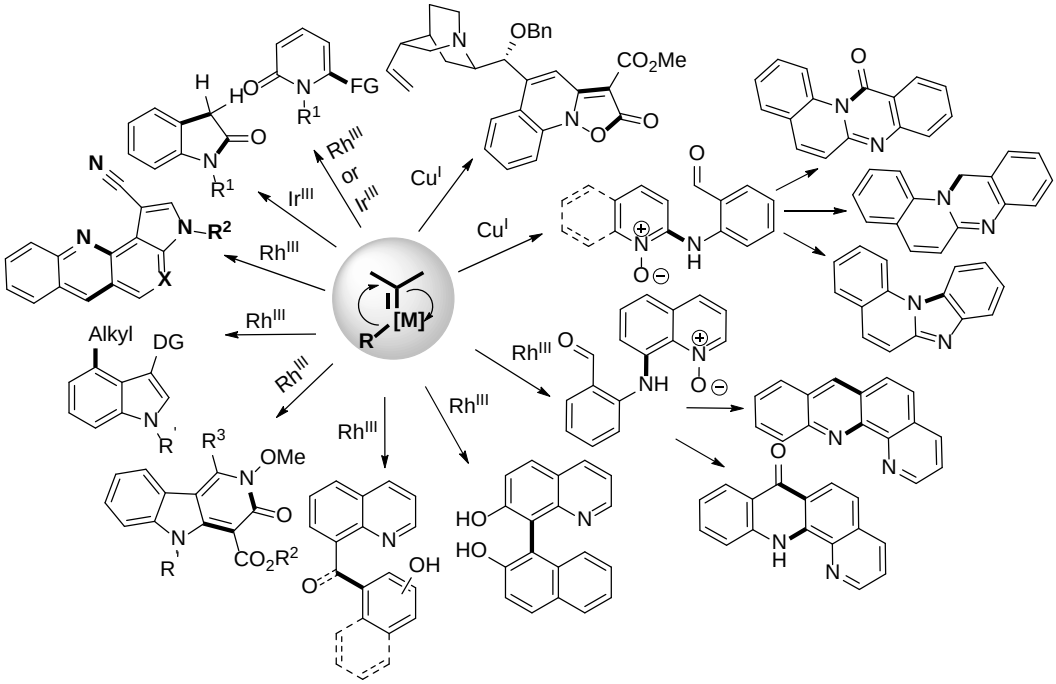
Abstract

Nitrogen-containing synthons like diazo compounds; azides etc. are valuable and versatile precursors for reactive intermediates like carbenes and nitrenes. Under transition metal catalyzed conditions, the formed metal carbene/nitrene intermediates undergo traditional reactions like X-H insertions, cyclopropanations, ylide formations, 1,2 shift, etc. Compared to the well studied classical reactions of them, directed C-H metalation, metal-carbene/nitrene formation followed by migratory insertion with suitable coupling partners has emerged recently.[1] In this presentation, regioselective alkylation, arylation and amidation of 2-pyridone scaffold will be discussed.[2] Furthermore, preparation of oxindole derivatives[3] and regiodivergent indole alkylation[4] and annulations[5] will be presented. Finally, the synthesis of 8-azaBINOL, benzophenanthroline, benzophenanthrolinone and extended organic π-conjugated systems on quinoline scaffold will be explored.[6-9]



Scheme: Straightforward construction of azaheterocycles using metallocarbenes and nitrenes

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Bio-Sketch of Speaker

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Education:

B.Sc.: Jadavpur University, Kolkata, India, 2002

M.Sc.: Jadavpur University, Kolkata, India, 2004 (Mentor: Prof. R. Ghosh)

Ph.D.: Indian Institute of Chemical Technology, Hyderabad, 2010 (Mentor: Prof. T. K. Chakraborty).

Postdoctoral Tenure:

- Max Planck Institute of Molecular Physiology, Dortmund, Germany. (June 2010-Sep 2013; Mentor: Dr. A. P. Antonchick)

Employment:

- **Associate Professor,** Indian Institute of Technology Kharagpur; Aug 2019–present.
- **Assistant Professor,** Indian Institute of Technology Kharagpur; Sep 2013–Aug 2019.

Fellowships/Honours:

- Associateship for the Indian Academy of Sciences (2019-2022)
- Max-Planck Postdoctoral Fellowship (2010-2013)

Specialization: Transition Metal Catalysis, Asymmetric Synthesis, Natural Product Synthesis

Current Research Interest: We are interested in the development of transition-metal-catalyzed step economic transformations using metallocarbenes and nitrenes via directed C-H metalation, metal-carbene formation followed by migratory insertion with suitable carbene and nitrene precursors. We investigate the late-stage modifications of various complex heterocyclic molecules in a catalytic way. Recently, we are working on the construction of *N*-PAHs in step-economic way.

Designed Negative Feedback from Transiently formed Catalytic Nanostructures

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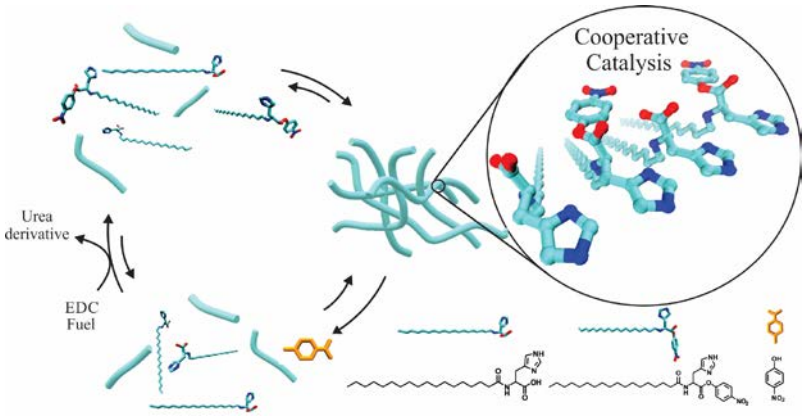
Abstract:
Structures in living systems manipulate the high energy ester bonds of chemical fuels to create dissipative assemblies which can access emergent functions such as catalysis. Highly dynamic and complex systems of microtubules undergo substrate driven change of conformation which leads to polymerization. Through this talk, I will show our recent results which demonstrate through a simple model system, the realization of a substrate driven dissipative self-assembled state by utilizing the catalytic effects of histidines on the kinetically stable ester bond.[1-3] Out of equilibrium state is achieved due to two distinct pathways both catalyzed by histidine, installed in the simple lipid based structure. Firstly, histidine facilitates the ester bond formation, which then rapidly coassembles to form a self-supporting gel. Also, out of equilibrium state is realized due to the emergence of cooperative catalysis by the proximal histidines in the assembled state, driving the second pathway and resulting in disassembly to sol. This simple system models the structural journey seen in microtubule formation, where the emergence of catalytic roles in assembled state results in the dynamic instability and disassembly of filaments. Further, I will share the latest data on temporal control of functional by these artificial transient systems.[3]

Figure:



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3. Bal, S.; Das, K; Ahmed, S.;, **Das, D*** Angew. Chem. Int. Ed. 2019 58 244
4. Kapil, N.; Singh, A.; Singh, M.; **Das, D*** Angew. Chem. Int. Ed. 2016 55 7772
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Invited Lecture (IL-07)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

Dr. Dibyendu Das
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IISER Kolkata

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Dibyendu Das is Assistant Professor in the Department of Chemical Sciences of Indian Institute of Science Education and Research (IISER) Kolkata. He received his MSc degree in Organic Chemistry at the University of Calcutta (India) (2005), PhD in Supramolecular Chemistry at Indian Association for the Cultivation of Science (Thesis 2010) and postdoctoral training at the Emory University. From Jan 2017, he is working in IISER Kolkata.

Invited Lecture (IL-08)
International Conference on Organometallics and Catalysis (ICOC 2020)

Asymmetric Ion-Pairing Catalysis with N-Heterocyclic Carbene

Joyram Guin *
School of Chemical Sciences
Indian Association for the Cultivation of Science (IACS), India
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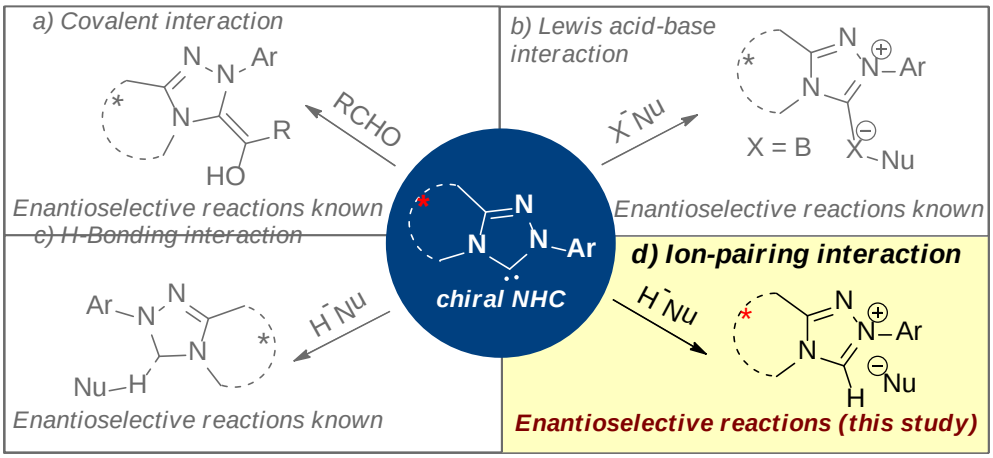
Abstract:
In the domain of asymmetric organocatalyst, chiral N-heterocyclic carbenes (NHCs) have received significant interest. The ability of NHC to activate diverse class of substrates via different modes of interaction is particularly intriguing.[1] Accordingly, asymmetric NHC-catalysis involving covalent interaction with substrates possessing activated carbonyl functional group (Scheme 1a),[2] Lewis acid–base interaction with silicon or born reagents (Scheme 1b)[3] and hydrogen bonding interaction with the substrates in the presence of a proton shuttle (Scheme 1c)[4] have been developed. Furthermore, attempts have also been made in developing asymmetric NHC-catalysis via ion-pair interaction with substrates utilizing the intrinsic Brønsted base[5] characteristic of NHCs without having much success. Very recently, our group has successfully demonstrated highly enantioselective organic transformations using NHCs as Brønsted base catalysts (Scheme 1d).[6] The reaction are expected to proceed through the catalytic formation of a chiral ion-pair comprising of the enolate and chiral azolium ion. Detailed reaction design, development, substrate scope and preliminary mechanistic investigations will be discussed during the lecture.



Scheme1: Different modes of asymmetric NHC-catalysis.

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Bio-Sketch of Speaker

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Dr. Joyram Guin obtained his PhD in 2007 at Westfälische Wilhelms- Universität, Münster in the group of Professor Armido Studer. After, he worked as postdoctoral fellow with Professor Jerome Lacour at University of Geneva (2008-2010) and with Professor Benjamin List at Max-Planck Institut für Kohlenforschung in Mülheim an der Ruhr (2010–2012). In 2013, he moved to Indian Association for the Cultivation of Science (IACS) as assistant professor. In 2017, he became associate professor at the School of Chemical Sciences, IACS. His research interests are focused on the development of new synthetic method based on radical chemistry, organocatalysis and transition-metal catalysis.

Awards:
Associate of the Indian Academy of Sciences (IASc)
Thieme Chemistry Journals Award (2014)

Invited Lecture (IL-09)
International Conference on Organometallics and Catalysis (ICOC 2020)

Effect of the Ancillary NHC Ligand in Ruthenium(II)-Catalyzed Organic Transformations

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Indian Institute of Technology Madras, Chennai - 600036
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Abstract: Ancillary ligands are known to play crucial roles in the catalytic activity of any metal complexes and their stereoelectronic parameters are normally regarded as important factors to tweak their properties and thus catalytic activity. Over the past few decades, *N*-Heterocyclic Carbenes (NHCs) have established themselves as an important class of ligand in various fields including homogeneous catalysis.[1] Although extensively utilized in catalysis, detailed study on the combined steric and electronic influence of an ancillary NHC ligand in transition metal catalyzed hydride transfer reaction, play decisive role in many important catalytic processes, are rather limited.[2] Detailed understanding of this type would definitely provide useful input for the future catalyst developments. To study such effects, we have synthesized a series of Ru(II)-complexes with either orthometalated $C_{NHC}\wedge C_{phenyl}$-bidentate NHC ligands or unsymmetrical chelating ligands where an imidazolylidene donor (ImNHC) is coupled to a pendant triazolylidene (tzNHC)/N-donor (Fig. 1). To understand the influence of ligand variations, all these complexes were applied in the transfer hydrogenation of unsaturated substrates as model hydride transfer reaction and observed that substantial tailoring of catalytic activity is possible based on their steric and electronic profiles.[3a-b] This fine tuning of activity can possibly be correlated with the electron-richness of the Ru(II)-center which was evident from the NMR and electrochemical studies. Further, these complexes also act as efficient catalysts for the alkylation of variety of substrates using alcohols.[3c]

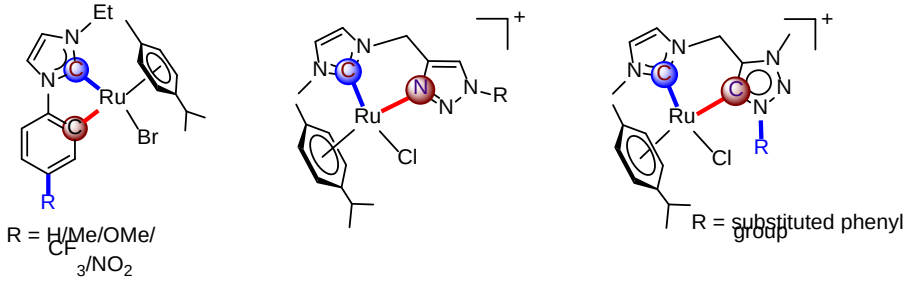

Figure 1: Ru(II)-NHC complexes used in this study.

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Invited Lecture (IL-09)

International Conference on Organometallics and Catalysis (ICOC 2020)

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After graduating from IIT Kharagpur in 2007, Dr. Rit has earned his doctorate degree in Organometallic Chemistry in 2011 from WWU Muenster, Germany. After that he was a post-doctoral researcher at RWTH Aachen, Germany for about 2 years and Marie-Curie post-doctoral fellow for one and half year at the University of Oxford. In December, 2015 he joined IIT Madras as an Assistant Professor and currently working on the synthesis and catalytic application of metal-NHC complex.

Invited Lecture (IL-10)
International Conference on Organometallics and Catalysis (ICOC 2020)

Searching of an alternative reactivity in the hydrogen bonding catalysis

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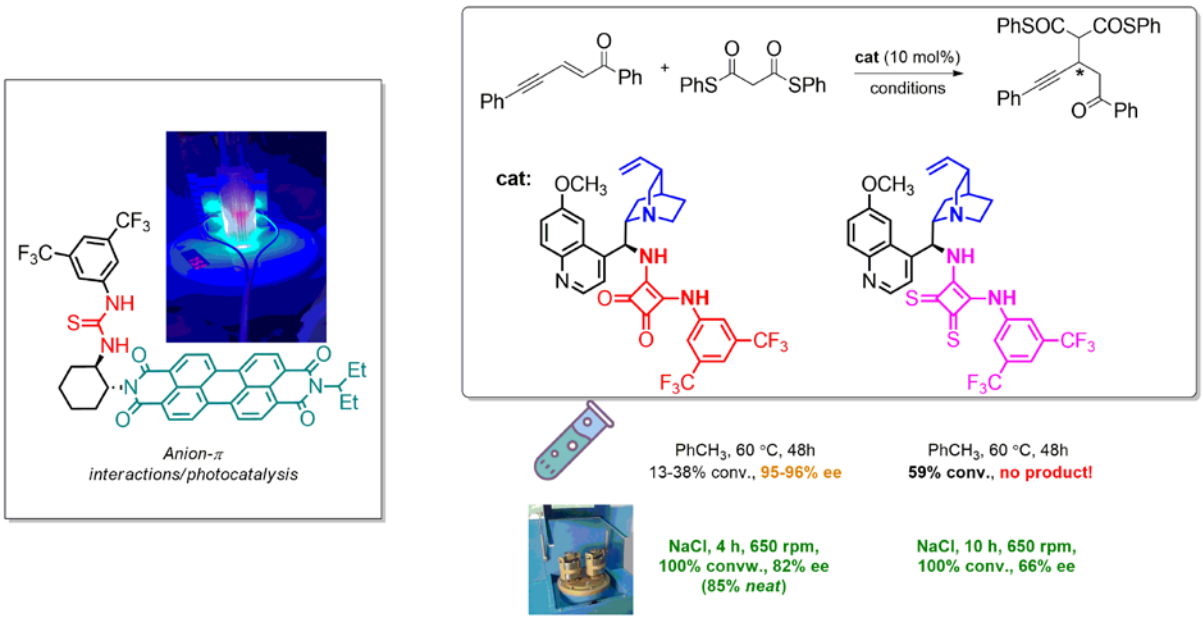
Abstract:
A bunch of factors could influence the reaction path. The way from the substrate to the product may diverge as a result of subtle conditions. In this light, catalysis is a perfect tool to create the desired reactivity or selectivity, including stereoselectivity. On the other hand, starting from the same compounds, different products could be available. In this short communication, the attempts to find an alternative reactivity in the organocatalyzed transformations will be covered. Focused on the *unorthodox interactions at work* [1], the presented results will be devoted to versatile hydrogen bond donors and their applications in the hydrophobic amplification processes [2], photochemical transformations and with the strong emphasis, in mechanochemistry [3].



Reactions performed in the absence of solvent provide a few conveniences from which the most promising is the possibility to achieve impossible or different reactivity in comparison to analogous transformations performed applying the standard conditions in solution.[4] Here, a different selectivity and reactivity patterns will be presented in the stereoselective formation of C-C bonds.

References and Notes:

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Invited Lecture (IL-10)

International Conference on Organometallics and Catalysis (ICOC 2020)

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Rafał Kowalczyk, at the early stage of career, worked on the asymmetric synthesis, stereodifferentation in NMR and electrophilic, metal-based complexes and their application in asymmetric catalysis. The latter approach was further developed with the group of Professor Jurczak (Institute of Organic Chemistry PAN, Warsaw), where the research was devoted to the application of the sterically biased chromium (III)-SALEN complexes in the stereoselective C-C bond formation and total synthesis of Centrolobine. When joined shortly after the group of Professor Carsten Bolm (RWTH Aachen University, Germany), he was working on the synthesis of fluorinated sulfoximines and sulfonimidamides. With the cooperation with the prof. Masahiro Miura group, he also worked on the direct copper-catalyzed sulfoximination of azoles involving activation of C-H bonds.

Currently, as an Associate Professor at the Wroclaw University of Technology, his work is focused on asymmetric catalysis, hydrogen bond donors, organic synthesis and mechanochemistry. Together with prof. Robert Góra (Theoretical Chemistry Group, Institute of Physical and Theoretical Chemistry, Wrocław University of Science and Technology) he is also involved with the understanding of the nature of hydrogen bonding and mechanisms of photochemical reactions.

N-Nitroheterocycles: Easily Accessible, Bench-Stable and Broadly Applicable Reagents for Catalytic Nitration

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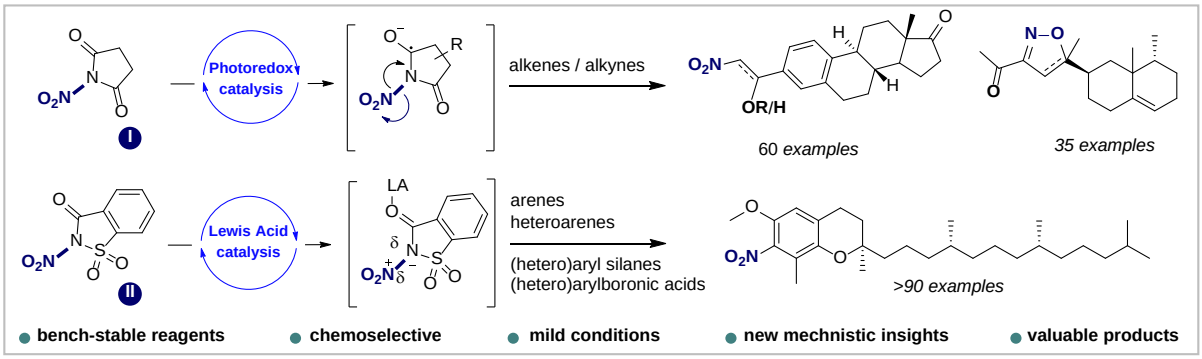
Abstract

Nitro compounds are essential constituents of drugs and intermediates in the synthesis of biorelevant molecules, agrochemicals and materials. The most frequently exploited synthetic method for the nitration of various carbon−hydrogen bonds involves the use of a mixture of concentrated nitric and sulphuric acid. This methodology is limited in its application in the synthesis of complex molecules, since such harsh conditions do not tolerate acid-sensitive functionalities, and results in numerous by-products. Herein, we report the design, synthesis and applications of one of the first, bench-stable non-metal based, organic nitrating reagents, which can be prepared from cheap, commercially available chemicals in one-step on a large scale [1,3]. These reagents act as a controllable source of both the nitronium ion using Lewis acid catalysis and the nitryl radical species using photoredox catalysis. In the first case, broad range of Lewis acids were found to be efficient catalysts to promote nitration through the direct or *ipso*-substitution reaction of aromatic and heteroaromatic compounds. Due to the reagent's excellent reactivity and the very mild and neutral conditions of methods, reactions exhibit an unprecedentedly broad substrate scope, and were successfully used for the nitration of various pharmaceuticals, agrochemicals and materials. Detailed mechanistic studies strongly support an electrophilic reaction pathway, which was found to proceed through a unique and highly ordered transition state. Furthermore, a single-electron reduction enables the formation of NO_2 radicals in a controlled and selective fashion under visible-light photocatalytic conditions, allowing access to a broad range of nitrated molecules such as nitroolefins, β-nitrohydrines and isoxazole derivatives [2].



Scheme: Novel class of nitrating reagents and their use in organic synthesis.

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Invited Lecture (IL-11)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Dmitry Katayev completed his Master of Science in Chemistry and Chemical Engineering at the Higher Chemical College of the Russian Academy of Sciences (Moscow) in 2008. He received his doctorate degree in chemistry at the University of Geneva (Switzerland) in end of 2012 under the supervision of E. P. Kündig. Awarded by the Swiss National Science Foundation (SNSF) fellowships, he pursued postdoctoral research with L. J. Gooßen at TU Kaiserslautern (Germany) and subsequently with A. Togni at ETH Zürich (Switzerland). Since early 2017, he is a Principal Investigator under Ambizione Fellowship funded by the SNSF at ETH Zürich (Switzerland). His research focuses on the development of novel classes of functional group transfer reagents that are used for the construction of various C−C and C−heteroatom bonds.

Design and Synthetic Applications of Rhodium-Enalcarbenes

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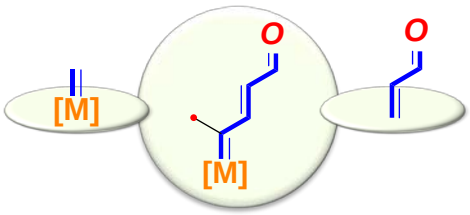
Abstract:
Metal-carbenes derived from diazo compounds are valuable reactive intermediate in a variety of carbene transfer reactions such as cycloadditions, ylide-reactions, rearrangements, σ-bond insertions (C-H, C-C, C-X, X-X) and cross-coupling reactions.[1] However, the discoveries from such metal-carbenes limited by the available classes of diazo substrates. To broaden the scope of the carbene chemistry, our group designed a new type of enal-functionalized carbenes derived from diazoenals.[2] This is the first example in which a privileged metal–carbene and the enal functionality are united allowing seamless integration of metal catalysis, and organocatalysis. This presentation highlights the design and synthetic applications of diverse enal-carbenes.

Figure:



enal-carbene
-Design
-New reaction development
-Synthetic applications

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Invited Lecture (IL-12)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Sreenivas studied M.Sc. (Chemistry) at the School of Chemistry, University of Hyderabad. Subsequently, in 2002 he received a Ph.D. in synthetic organic chemistry under the guidance of Prof. Goverdhan Mehta. He held postdoctoral positions at the Rutgers University and Florida State University, USA. Later, he joined Cambrex, USA, where he developed a GMP process for the anticancer drug Docetaxel. After a brief stint at ILS, he joined as the Assistant Professor at the Indian Institute of Science Education and Research, Bhopal. His research interest includes the design and synthetic applications of new metal-carbenes.

Main Group Lewis Acids for Hydrosilylation

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Abstract:
Curiosity driven research in the isolation of reactive main group cations has led us explore their potential as Lewis acid catalysts. Lewis acidic cationic compounds of magnesium,[1] zinc,[2] aluminum,[3] antimony and bismuth [4] have been prepared in our group. These compounds have been demonstrated as successful catalysts in the hydrosilylation of alkenes, alkynes, aldehydes, ketones and carbon dioxide. Mechanistic investigations by experiments and theoretical investigations have revealed the role of the active species in hydrosilylation reactions.

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Invited Lecture (IL-13)

International Conference on Organometallics and Catalysis (ICOC 2020)

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Our research interests are in the in the frontier areas in main group chemistry. While the primary focus is on understanding the structure and bonding in reactive main group compounds, stabilization of unusual coordinate modes, activation of inert chemical bonds and Lewis acid catalysis. Ajay Venugopal obtained his doctoral degree in 2008 from the University of Muenster, Germany, under Prof. Norbert W. Mitzel. He later moved to SINTEF Materials and Chemistry in Oslo, Norway, to work with Dr. Richard H. Heyn and Prof. Mats Tilset on gold-catalyzed C-H bond activation. In 2010, he received an Alexander von Humboldt fellowship to work with Prof. Jun Okuda at RWTH Aachen, Germany, on lanthanide hydrides.

Towards Sustainable C–H Bond Functionalization Reactions

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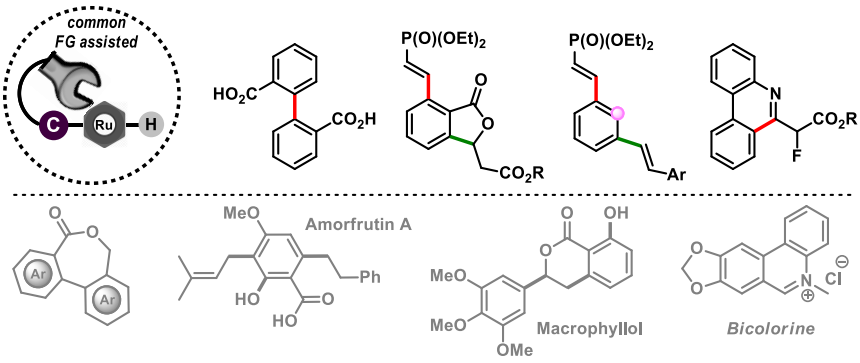
Abstract:
Development of sustainable synthetic strategies to assemble molecular complexity from simple precursors is a continuous enterprise in contemporary organic chemistry. In this context, transition metal catalyzed functionalization of otherwise inert C–H bonds via exploitation of common organic functional groups (FGs) is highly alluring as they are synthetically valuable, readily accessible, and also avoid obstruction associated with the installation/removal of the directing group (DG).[1] In this area, we have introduced the use of carboxylic acid functionality as a weakly coordinating directing group for position selective styrylation, annulation, dimerization, and chalcogenation with versatile ruthenium catalysts.[2] Recently, we have unfolded free amine as a directing group in cross-ring-annulation (CRA) reaction under Ru-catalysis.[2b] The detailed mechanistic insights of C–H ruthenation step enabled hydroarylation of alkenes with concomitant decarboxylation *en route* to formal *meta*- and *para*-functionalization and one-pot twofold unsymmetrical olefination of arenes.[2a,g] The developed strategies can be harnessed to synthesize biologically important scaffolds and natural products. This presentation will provide an overview of some recent advancement in our laboratory on transition-metal catalyzed selective C–H bond functionalization of arenes.



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Invited Lecture (IL-14)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Mahiuddin Baidya studied chemistry at Indian Institute of Technology Kanpur (IITK), India. He obtained his PhD in 2009 from Ludwig-Maximilians-Universität München (LMU), Germany under the supervision of Prof. Herbert Mayr. After postdoctoral studies with Prof. Hisashi Yamamoto at The Universality of Chicago, USA and Molecular Catalyst Research Center in Japan with JSPS fellowship, he moved in 2014 to Indian Institute of Technology Madras (IITM) as assistant professor, and was promoted to associate professor in 2018.

His research interest includes the development of novel concept on transition-metal-catalysis, organocatalysis and visible-light photocatalysis for organic synthesis.

He is a recipient of INSA-Young Scientist Medal (2017), NASI-Young Scientist Platinum Jubilee Award (2017), Institute Research & Development Award (IRDA, early career level, 2018) and also became an Associate of the Indian Academy of Sciences (IAS) in 2017.

Functional Organic Radicals and Redox Cascades

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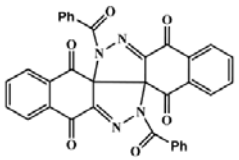
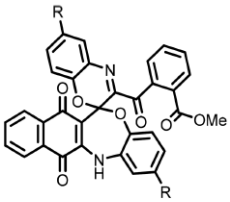
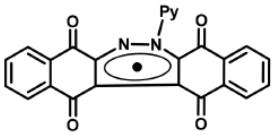
Abstract:
Organic radicals that exhibit diverse redox activity in biology and catalytic chemistry are significant entities in chemical science. The role of radical intermediates has a paramount importance in several reactions of organic chemistry. Thus stabilization of radical intermediates and applying them purposely are a challenge in chemistry. Stabilization of organic radical was successful in coordination complexes of transition metal ions and in this context several types of transition metal complexes of organic radicals were isolated and characterized by experimental and theoretical investigations. Various types of reactivities of the coordinated radicals were explored. Notable of them are that the organic radicals coordinated to transition metal ions expand the redox activities of the central metal ions, they participate in multi-electron transfer reactions that are not expected considering the redox activity of the metal ion only and they exhibit catalytic activities as documented in several aspects. In this event, I will talk on organic radicals promoted redox cascades furnishing indazolo − indazole, spiro oxazine-oxazepine, *o*-phenylenediimine derivatives and 1,2-benzodiazinyl radicals (Chart 1) and their molecular and electronic structures and activities.[1-4]

Chart 1







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Invited Lecture (IL-15)

International Conference on Organometallics and Catalysis(ICOC 2020)

Bio-Sketch of Speaker

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Research Interest

Modeling of functional metal-organic fragments, particularly coordination complexes of organic radicals and study of their role in multi-component electron transfer, aromatic ring cleavage, C-H activation, redox cascade, concerted proton-electron transfer (CPET) reactions, mixed valency and catalysis

Experimental Approach and Expertise: Syntheses, Cyclic Voltammetry and Spectro-electrochemistry, EPR Spectroscopy and Simulation, Single Crystal X-Ray Crystallography

Theoretical Approach: Density Functional Theory (DFT), Broken Symmetry (BS) DFT and TD

Contribution: Foundation of a Research Laboratory at the R. K. Mission Residential College with the following sophisticated equipment: (i) Single Crystal X-Ray Diffractometer (ii) EPR spectrometer (iii) ESI and GC Mass Spectrometer (iv) Electrochemistry and Spectro-electrochemistry System and (v) facilities for DFT Calculations

Awarded

- Alexander von Humboldt Research fellowship
- Max-Planck-Society research fellowships
- Senior Alexander von Humboldt Research fellowship
- Prof. D. Nasipuri Memorial Award from Chemical Society of India and
- Elected as a Fellow of West Bengal Academy of Science and Technology (WAST)

Publications

Published more than 85 articles in the area of coordination chemistry of organic radicals in the journals of international repute

Invited Lecture (IL-16)
International Conference on Organometallics and Catalysis (ICOC 2020)

Construction of Natural and Unnatural Biologically Significant Carbocycles from *p*-Quinone Methides

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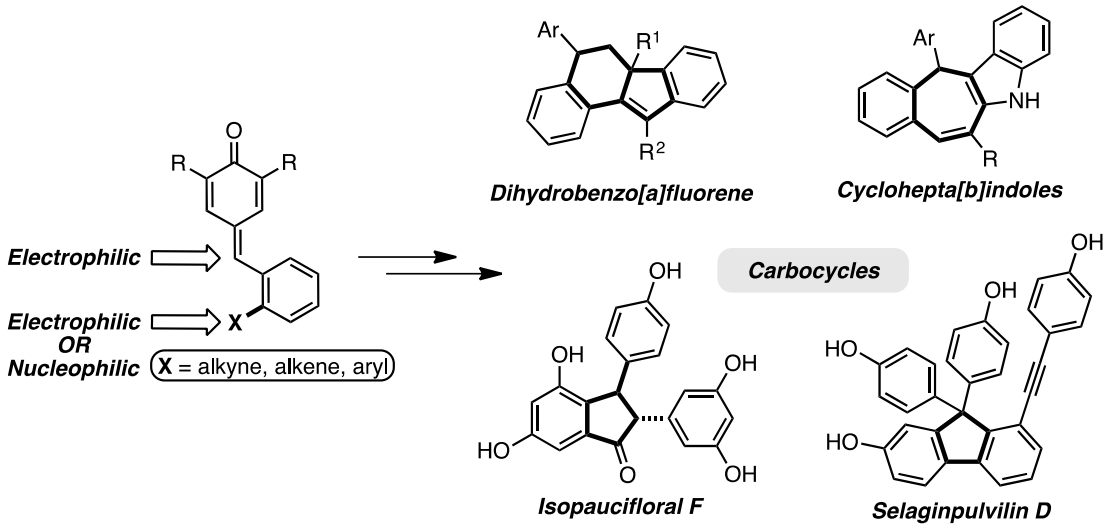
Abstract:
The unique reactivity profile of *p*-quinone methides (*p*-QMs) has been explored in 1,6-conjugate addition reactions[1] including enantioselective transformations.[2] In the past few years, our research group developed several synthetic transformations of *p*-QMs through 1,6-conjugate addition reactions leading to unsymmetrical diaryl- and triarylmethane derivatives.[3] In addition, a few other synthetic methods have been developed in our lab to access biologically significant carbocycles and heterocycles utilizing *p*-QMs as synthons.[4] A part of this ongoing research will be discussed in the talk.



References and Notes:

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2. For reviews: (a) Li, W.; Xu, X.; Zhang, P.; Li, P. *Chem. Asian J.* **2018**, *13*, 2350. (b) Caruana, L.; Fochi, M.; Bernardi, L. *Molecules* **2015**, *20*, 11733.
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Invited Lecture (IL-16)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Ramasamy Vijaya Anand obtained Ph.D. in synthetic organic chemistry from the Indian Institute of Technology Kanpur in 2003. Subsequently, he moved to Glasgow, UK to take up a postdoctoral position at the University of Strathclyde, where he worked for two years. He held another postdoctoral stint at the Texas A&M University, College Station, USA prior to joining Dr. Reddy's Laboratories at Hyderabad in 2006. During his three years of stay at Dr. Reddy's, he served as a group leader in 'complex molecules development' team and involved in developing cost-effective route to a few anti-HIV agents. In 2010, he moved to IISER Mohali, where he is currently working as an associate professor. His research interests include nucleophilic carbenes catalyzed enantioselective transformations, electrophilic annulation reactions leading to heterocyclic systems, and synthesis of natural and unnatural biologically active compounds.

Invited Lecture (IL-17)
International Conference on Organometallics and Catalysis (ICOC 2020)

Convenient Access to Pyrrolinium Cations: A Synthon for Carbon Based Radicals

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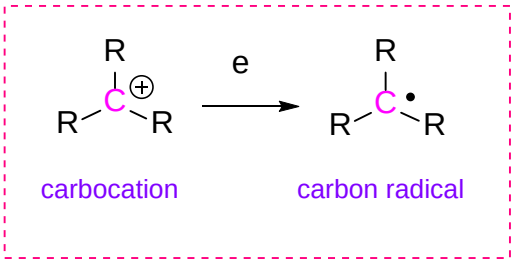
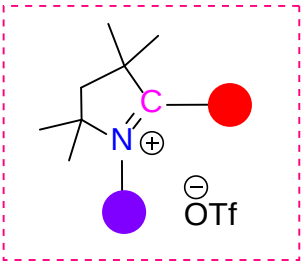
Abstract
Radicals play an important role in bond-forming and bond-breaking processes.[1] In organic chemistry, however, carbon-centred radicals are usually observed as rather short-lived intermediates. In recent years there have been reports on the isolable carbon based delocalized and localized radicals.[2] One of the synthetic route for the generation of carbon based radicals could be the 1-e reduction of corresponding carbocation.





In this talk I will discuss the convenient synthetic route for the syntheses of different kinds of pyrrolinium cations, which we have used for the synthesis of carbon centre based localized and delocalized radicals.[3]

References:

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Invited Lecture (IL-17)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Dr. Anukul Jana obtained his Ph.D. in 2009 from University of Göttingen, Germany under the guidance of Professor Herbert W. Roesky. His doctoral thesis focused on the chemistry of compounds with low-valent Group 14 elements. He did his first postdoctoral research work as a Alexander von Humboldt fellow in the group of Professor Paul Knochel, Ludwig-Maximilians-Universität, Germany. Later on he moved to pursue his second post doctoral research in the group of Professor David Scheschkewitz, Universität des Saarlandes, Germany. In March 2014, Dr. Anukul Jana started his independent career at TIFR Hyderabad. His current research interest is mainly in the chemistry of low-valent low-coordinate Group 13-15 elements.

Bio-Sketch of Speaker

Dr. Huw M. L. Davies
Asa Griggs Candler Professor of Chemistry

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Huw M. L. Davies was born in Aberystwyth, Wales, UK. He received his B. Sc. degree from University College Cardiff, Wales (1977) and his Ph. D degree from the University of East Anglia (1980). After a post-doctoral position at Princeton University (1980-1983), he joined the faculty at Wake Forest University (1883-1995). After being promoted to full professor he moved to the University at Buffalo, the State University of New York (1995-2008) where he held the positions of UB Distinguished Professor and Larkin Professor of Organic Chemistry. In 2008 he moved to Emory University as the Asa Griggs Candler Professor of Chemistry.

Professor Davies' research emphasizes the development of new enantioselective synthetic methods and their applications in total synthesis and drug discovery. A major current theme of his program is catalytic asymmetric C–H functionalization by means of rhodium-carbene induced C–H insertion. He is currently the Director of the NSF Center for Chemical Innovation for Selective C-H Functionalization, which brings together 23 faculty members from 15 universities.

Professor Davies is actively involved in the chemical community, having served as the Executive Officer of the 2003 National Organic Symposium, the 2005 Program Chair of the Gordon Conference on Heterocyclic Compounds, the 2005 Chair of the Organic Division of the American Chemical Society, and Co-Organizer of the ACS Organic Division Assistant Professor Symposium at the Fall ACS meeting since 2006. He is an Associate Editor for Chemical Society Reviews and has been as Associate Editor of Organic Reactions (2005-2010) and Organic Syntheses (2008-2016). Recent awards include the American Chemical Society Cope Scholar Award (2005), Fellow of the Royal Society of Chemistry (2007), Fellow of the American Chemical Society (2009), Fellow of the American Association for the Advancement of Science (2012), 2013 eEROS Reagent of the Year Award, Fellow of the National Academy of Inventors (2015), the Alexander von Humboldt Foundation Research Award (2017), the Paul N. Rylander Award (2018) and the ACS Herbert C. Brown Award for Creative Research in Synthetic Methods (2019).

Oxygen Driven Fragment Coupling by Activation of C-H, N-H, and O-H Bonds

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Department of Chemistry
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Abstract:

Nature uses oxidative couplings to construct carbon-carbon, carbon-oxygen, and carbon-nitrogen bonds with a high degree of efficiency. Surprisingly, few laboratory equivalents are as selective or as efficient as the biological versions. The use of parallel microscale screening to discover selective and efficient catalysts for such processes using oxygen as the terminal oxidant will be discussed. The unexpected outcomes obtained highlight the value of interrogating large numbers of rationally selected variables under the umbrella of general hypothesis.

The development of selective catalytic processes for, phenol coupling, asymmetric phenol coupling, enol coupling, N-arylation, and alkyl C–H activation that utilize oxygen as the terminal oxidant will be discussed. Applications in total synthesis of hypocrellin, bisoranjidiol, honokiol, and chaetoglobin will be presented. Studies on the mechanisms of these transformations will be described with the goal of understanding the governing principles and how they might be used to discover further new transformations. Finally, the use of machine learning to extract mechanistic insight for the catalysts array will be discussed.

Invited Lecture (IL-19)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Marisa Kozlowski received an A. B. in Chemistry from Cornell University in 1989 and a Ph.D. from the University of California at Berkeley in 1994 for work on the rational design of enzyme inhibitors under the direction of Paul Bartlett. After studying asymmetric catalysis in the laboratories of David A. Evans at Harvard University as a National Science Foundation postdoctoral fellow, she joined the faculty at the University of Pennsylvania and currently holds the rank of Professor of Chemistry.

The major focus of Professor Kozlowski's research is the development of new catalytic methods for efficient organic synthesis using computation and high throughput screening. Professor Kozlowski's contributions have been recognized by a DuPont Young Investigator Award in 1998, an NSF CAREER Award in 2001, an Alfred P. Sloan Research Fellowship, the Kahn Award for Distinguished Teaching at the University of Pennsylvania, an American Cancer Society Beginning Research Scholar Award in 2002, the Philadelphia Organic Chemists' Club Award in 2010, election as a Fellow of the American Association for the Advancement of Science in 2012, the Philadelphia ACS Section Award in 2012, and election as an American Chemical Society Fellow in 2013. In addition to over 170 independent publications, Professor Kozlowski coauthored with Professor Patrick Walsh the book "Fundamentals of Asymmetric Catalysis", available from University Science Books. She has served in several leadership roles for the Organic Division of the American Chemical Society and on numerous study sections including a term as Chair of the American Cancer Society CDD Study Section. She is currently an Associate Editor for the *Journal of Organic Chemistry*.

Organometallic Catalysis for Energy Storage and Sustainable Synthesis

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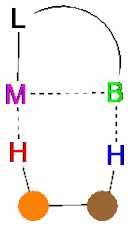
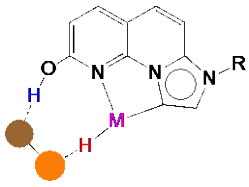
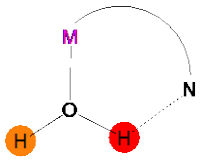
Abstract:
Synergic participation of two or more chemical functionalities in a catalyst has been credited to facilitate a difficult chemical process. Synthetic catalysts are designed where a cooperating-ligand actively participates in bond–activation process and undergoes reversible chemical transformation to make the catalytic process efficient and selective. Carefully designed ligand scaffolds, which hold a metal ion and simultaneously offer a proton-responsive unit, have been devised for water activation, hydrogenation and dehydrogenation reactions. This talk would focus on the scope of bifunctionality in organometallic catalysis with relevant examples.







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Invited Lecture (IL-20)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Jitendra Bera received M. Sc. from University of Kalyani in 1993 and Ph. D. from Indian Institute of Science, Bangalore in 1999. After a couple of postdoctoral stints at Purdue University and at Texas A&M University, he joined the faculty at IIT Kanpur in 2003, where he is currently serving as HAG Professor. He is elected fellows of three National Academies (FASc, FNASc, FNA). He recently received the J C Bose National Fellowship. His research in the field of Organometallic Chemistry has earned him several awards and recognitions including Outstanding Investigator Award (2015) by the Department of Atomic Energy (DAE), Swarnajayanti fellowship (2009) and Ramanna Fellowship (2007) by the Department of Science and Technology (DST), and Bronze medal (2012) by Chemical Research Society of India (CRSI). He is the recipient of the C. N. R. Rao National Prize (2018) in Chemical Sciences. He is currently serving as an Associate Editor, Applied Organometallic Chemistry (Wiley), Member: Editorial Advisory Board of Organometallics (American Chemical Society), Member of the International Advisory Board of the International Conference in Organometallic Chemistry (ICOMC). Bera's research interests span synthetic, structural and mechanistic organometallic chemistry and addresses energy, environmental and sustainability aspects of chemical synthesis.

Frustrated Lewis Pairs and Main group Catalysis

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Abstract:
We have previously exploited Frustrated Lewis pair (FLP) chemistry for the activation of H_2, hydrogenation catalysis and the capture of small molecules.[1] More recently we have uncovered evidence of both heterolytic and homolytic reactions for select FLPs affording either ionic or radical reaction pathways.[2] The access to radical pathways has been extended to develop novel air stable main group derived radicals as well as one-electron FLP chemistry.[3] Other efforts in expanding this concept, have focused on the activation of strong bonds. Specifically, we are interested in developing reactions of main group systems with N_2 and N_2-surrogates[4] as well as C-f bonds.[5] The latter efforts have led to the discovery of a series of main group Lewis acids that are capable of stoichiometric and catalytic activation of C-F bonds, providing highly selective protocols for $C(sp^2)$-$C(sp^3)$ and $C(sp^3)$-$C(sp^3)$ couplings that are complementary to traditional metal-based protocols for cross coupling. The further potential of these and related main group reagents in synthetic and catalytic synthetic chemistry is considered.

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Invited Lecture (IL-21)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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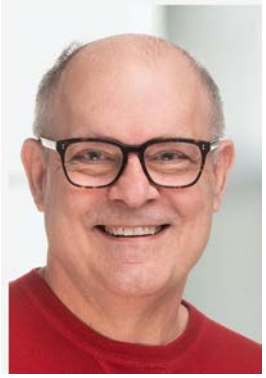

Doug Stephan, born in Hamilton, graduated with his BSc at McMaster (1976) and completed his PhD at UWO (1980). He then held a NATO PDF at Harvard, before beginning his independent career at the University of Windsor (1982). He was promoted to Associate Professor (1985), full Professor(1992) and named a NSERC Industrial Research Chair (2001), University Professor (2002) and Canada Research Chair(2005). In 2008 he moved to the University of Toronto as a Professor and Canada Research Chair, In 2018, he was appointed University Professor (top 1% of faculty at U of T). He was an Associated Editor for Chem. Soc. Rev. for 6 years and served as the Chair of the editorial board for a further 4 years.

While a highly successful world-leading researcher in inorganic chemistry/catalysis prior to his move to University of Toronto, the impact of his work exploded since the move. In articulating the concept of "frustrated Lewis pairs (FLP)" in 2006 Stephan established himself as the founder of the field of FLP chemistry. The impact of Stephan's work is clear, with research over 32000 citations to Stephan's work. Stephan has received recognition for his work including the 2001 Alcan Award (Canadian Society for Chemistry). an Av Humboldt Foundation Senior Research Award (2002), NSERC Synergy Award (2003), Ciapetta Lectureship Award (2004, North American Catalysis Soc.) and the LeSueur Memorial Award (2005, Canadian Soc. Chemical Industry). He was appointed as a Fellow of the Royal Society of Canada in 2005, awarded a Killam Research Fellowship (2009-2011), a Senior Award re-invitation from the Humboldt Foundation(2011), the Ludwig Mond Award and Lectureship (Royal Soc. Chemistry UK, 2012) and the 2013 H.M. Tory Medal from the Royal Society of Canada. He was elected a Fel[1a]low of the Royal Society (2013, London). In 2014, he was elected a Corresponding Member of North-Rhein-Westfaelia Academy of the Sciences and Arts (Germany) and awarded the Applied Catalysis Award (Royal Society of Chemistry, UK), Canadian Green Chemistry and Engineering Award and Chemical Institute of Canada Medal. In 2015, he was a Distinguished Adjunct Professor, King Abdulaziz University and in 2016-2019 was named an Einstein Visiting Fellow at the Technical University of Berlin. For each of the last 6 years, he has been named to the Thomson Reuters Highly Cited List, and in 2015 named to the List of World's Most Influential Scientific Minds. In 2019, he was awarded the NSERC of Canada J.C. Polanyi award and the EW.R. Steacie Award from the Chemical institute of Canada.

Catalytic methane functionalization with Pt complexes

Jennifer A. Love
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Abstract:

The catalytic functionalization of unreactive small molecules such as methane via C-H activation is a long-standing goal in organometallic chemistry. Late transition metals, such as platinum, have been shown to be quite effective in breaking strong C-H bonds. Recently, we have been exploring the feasibility of catalytic methane functionalization employing aryl halides as oxidants. Key challenges include the unreactive nature of Pt(II) toward intermolecular aryl halide oxidative addition, and the challenges with balancing the preference for Pt(II) versus Pt(IV) oxidation states. We have recently discovered Pt(II) complexes that are capable of intermolecular oxidative addition of aryl halides under ambient conditions. We have also designed and developed new hemilabile P,N ligands that facilitate both oxidative addition and reductive elimination relative to more conventional N,N or P,P ligands. Notably, only the P,N ligands with significant steric bulk at phosphorus were capable of forming the strained chelates. These results will be discussed in the context of our ongoing efforts to catalytically functionalise methane.

Invited Lecture (IL-22)

International Conference on Organometallics and Catalysis (ICOC 2020)

Biosketch of Speaker

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Education

2003–Present, (UBC)
2000-03, NIH Post-Doctorate (Caltech, Prof. R.H. Grubbs)
2000, Ph.D. (Stanford U., Prof. Paul Wender)
1994, B.Sc. (Allegheny College)

Awards and Honours

2009: Killam Teaching Prize
2008: AstraZeneca Canada Award in Chemistry
1998: Stanford University Centennial Teaching Award
1993: Phi Beta Kappa

Improving Efficiency via Catalysis and Multicatalysis

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Abstract:

Oxidative addition and reductive elimination are two fundamental steps common to many different catalytic reactions. Insertion into C-X bonds is particularly prevalent as one of the first steps in a catalytic cycle.

We have been exploring the synthetic potential associated with reversible oxidative addition into carbon-halogen bond and recently developed a palladium and nickel catalyzed carboiodination.[1] This lecture will describe the scope and limitations of the reaction including recent work that has expanded the scope. [2-3]

We have also been exploring the value of combining catalysts and substrates in a multicomponent multicatalyst strategy $(MC)^2R$.[4] Recent advances will be presented.

An efficient route to enantiomerically enriched heterocycles and carbocycles has been realized using borylcupration as a key step. We will present our recent work in this field.[5]

References

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3. Marchese, A.; Lind, F.; Mahon, A.E.; Yoon, H. "Forming Benzylic Iodides via a Nickel Catalyzed Diastereoselective Dearomative Carboiodination Reaction of Indoles" *Angewandte Chemie International Edition* **2019**, *58*, 5095-5099.

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Invited Lecture (IL-23)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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EDUCATION

B.Sc.	University of Guelph, 1981
Ph. D.	University of Wisconsin-Madison (Barry M. Trost)
Postdoctoral Fellow	Harvard University (David A. Evans)

ACADEMIC CAREER

1987-1998	Assistant to Professor, University of Toronto
1998-present	AstraZeneca Professor, University of Toronto
2012-present	University Professor, University of Toronto
2013-2023	J.B. Jones Distinguished Professor

QUALIFICATIONS AND AWARDS

(1) Officer of the Order of Canada, O.C. (2014)
(2) D.Sc. *honoris causa*, University of Guelph (2016)
(3) Faculty Award, University of Toronto (2016)
(4) CIC Medal (2013)
(5) Killam Research Fellow (2013)
(6) Pedler Medal, RSC (2011)

RESEARCH INTERESTS

Development of new synthetic reactions and strategies using metal catalysts.

Electrochemical Oxidation of Strong C-H bonds

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Abstract:
Scalable oxidation of unactivated C-H bonds, the most ubiquitous structural motifs in organic chemistry, remains a challenge. Such oxidations are typically performed using metal complexes together with oxygen-atom transfer reagents such as iodosylbenzene, peracids, and hydrogen peroxide. A lot of success has been demonstrated by the use of biomimetic iron complexes together with oxygen transfer agents such as hydrogen peroxide and/or sodium hypochlorite, which leads to the formation of the high valent oxoiron(V) intermediate. This oxoiron(V) intermediate has been shown to oxidize unactivated C-H bonds with high selectivity. However, the operational difficulties and formation of side products from the reactive oxidants limit their scalability. We have shown earlier that the active oxoiron(V) species can also be electrochemically generated *via* electrochemical proton-coupled oxidation (PCET) of the starting Fe(III)-OH_2 complex. Electrochemical oxidation of Fe(III)-OH_2 complex would bypass and need to chemical oxidants, as the reaction would be coupled to proton reduction at the cathode to generate H_2 as the sole product. In the lecture, I will discuss the electrochemical formation of oxoiron(V) by electrochemical PCET and then its use for the subsequent oxidation of unactivated C-H and C=C bonds to formed oxygenated products. The selectivities observed far exceeds the recent reports of electrochemical C-H oxidation using simple redox mediators such as quinuclidine.

References and Notes:

1. Baran, P. e*t al. J. Am Chem. Soc.* **2017**, 139, 7448

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Invited Lecture (IL-24)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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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, he joined NCL as a scientist in December 2006 where he was a Senior Scientist in the Chemical Engineering Division. He has recently moved to IISER-Kolkata in 2016 as an Associate Professor to the Department of Chemical Sciences. He is an inorganic chemist by training and works in the area of bio-inspired catalysis and materials.

Design, Synthesis and Functionalization of Imidazoheterocycles

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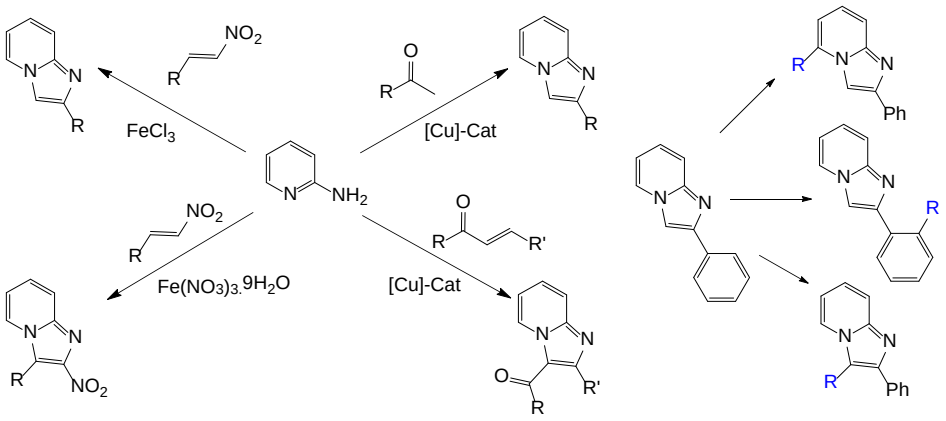
Abstract:

Heterocyclic compounds have gained a great deal of attention as majority of the drugs contain heterocycles and these plays a vital role in the society. So the developments of new synthetic strategies for heterocycles are prime targets of the organic chemists over the years. Imidazopyridine is one of the important fused bicyclic 5–6 heterocycles and it is recognized as "drug prejudice" scaffold due to its wide applications in medicinal chemistry. This scaffold is the constituent of various marketed drug like zolpidem, alpidem, zolimidine, necopidem, saripidem etc. In this lecture I will discuss our recent works on sustainable synthesis of imidazo[1,2-*a*]pyridines,[1] and some other heterocycles[2],[3] from 1,3-binucleophiles and further functionalization at different positions.



Synthesis and functionalization of Imidazo[1,2-*a*]pyridines

References and Notes:

1) (a) Bagdi, A. K.; Santra, S.; Monir, K; Hajra, A. *Chem. Commun.* **2015,** *51***,** 1555; (b) Monir, K.; Bagdi, A. K.; Ghosh, M.; Hajra, A. *Org. Lett.* **2014**, *16*, 4630; (c) Bagdi, A. K.; Rahman, M.; Santra, S.; Majee, A.; Hajra, A. *Adv. Synth. Catal.* **2013**, *355*, 1741; (d) Mandal, S. and Hajra, A. *J. Org. Chem.*, ***2017***, *82*, 4504.

2) (a) Rahman, M.; Bagdi, A. K.; Mishra, S.; Hajra, A. *Chem. Commun.* **2014**, *50*, 2951; (b) Dey, A.; Ali, A.; Hajra, A. . *J. Org. Chem.*, **2017**, *82*, 4812.

3) (a) Mitra, S.; Hajra, A. *Org. Lett*, **2014**, *16*, 5652; (b) Mishra, S.; Monir, K.; Mitra, S.; Hajra, A. *Org. Lett*, **2014**, 16, 6084; (c) Mondal, S.; Hajra, A. *Org. Lett*, **2017**, *19*, 3751; (d) Samanta, S.; Mondal, S.; Ghosh, D.; Hajra, A. *Org. Lett*, **2019**, *21*, 4905.

Invited Lecture (IL-25)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Alakananda Hajra graduated (M.Sc) from the Department of Chemistry, Indian Institute of Technology, Kharagpur India in 1998. After completing his Ph.D in 2002 under the supervision of Prof. B. C. Ranu from Indian Association for the Cultivation of Science (IACS), Kolkata he joined in SUNY at Albany, USA as a postdoctoral research fellow with Prof. Frank M. Hauser (2002-04). He was also a JSPS research Fellow in the University of Tokyo and worked with Prof. Eiichi Nakamura from November 2004 to May, 2006. He also worked with Prof. N. Yoshikai, NTU, Singapore for one year (2011-2012) as a visiting scientist. His research interests are the development of new synthetic methodologies and green synthetic procedures. He has published in more than 150 peer-reviewed articles with 6000 citations, giving him a *h*-index of 38. He has received "**Prof. D. K. Banerjee Memorial Lecture Award**" for the year 2015 from Indian Institute of Science and "**CRSI Bronze Medal Award**" for the year 2018.

Invited Lecture (IL-26)
International Conference on Organometallics and Catalysis (ICOC 2020)

Group 2 Metal Initiators as highly active and iso-selective catalysts for ROP of cyclic esters and amide

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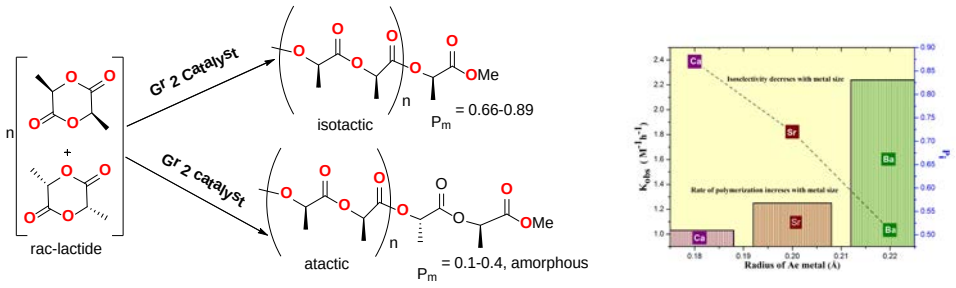
Abstract:
The current focus of a number of research group worldwide is on developing a distinct well-defined single-site catalyst that can control the stereochemistry of polyesters, whose mechanical properties and degradation profile may be fine-tuned, and thermal stability and crystallinity may be escalated, to produce a well-regulated molecular weight (M_n) and low polydispersity (PDI) polymer. The polymerization of *rac*-LA may produce either (i) an isotactic or (ii) a heterotactic PLA and atactic PLA, following a homochiral and heterochiral preference, introducing stereo irregularity in PLA. Isotactic PLAs obtained through the ROP of the enantio-pure L-lactide (L-LA) and D-LA have higher melting points (T_m) and modulus than atactic PLAs. Using an alternative approach in which an easily accessible achiral catalyst can promote stereoselective transformations by adopting chirality in the propagating step by chain-end bound to the catalyst in a chain-end controlled mechanism. This strategy is advantageous, as it averts the need for regenerated chiral precursors and rationalizes catalyst modifications to influence stereochemical outcomes.
In this presentation, synthesis of a series of alkali and alkaline earth (Ae) metal complexes supported by amidophosphin-chalgen/borane ligands and their exploitation in ring-opening polymerization (ROP) of *rac* lactide (*rac*-LA) and ε- caprolactone (ε-CL) at room temperature to achieve stereo control polymer will be presented.

Figure: 1. Ring-opening polymerization (ROP) of *rac*-LA by group 2 metal catalysts.



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Invited Lecture (IL-26)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Tarun K. Panda studied his Master of Science in Chemistry from IIT, Kanpur in 2002 and received his Dr. rer. nat from Freie Universität Berlin, Germany in 2005 under the supervision of Prof. Dr. Peter W. Roesky in the area of organometallic chemistry. Dr. Panda joined the working group of Prof. Dr. Matthias Tamm at Technische Universität Braunschweig, Germany as a postdoctoral fellow in 2006. He was awarded Japan Society for the Promotion of Science (JSPS) postdoctoral fellowship in 2008 to work with Prof. Kazushi Mashima in Graduate School of Engineering, Osaka University, Japan. In 2010, he returned to India to join in the Department of Chemistry, Indian Institute of Technology Hyderabad (IITH) India as Assistant Professor. He was promoted to Associate Professor in 2015 and since May 2019, he is holding the position of Professor at the same Institute. His principal research interests include the development of well-defined earth abundant, non-toxic and environmental benign metal complexes using the non-cyclopentadienyl based ligands and their exploitation in homogeneous catalysis under ambient reaction condition.

Publications:

1) Harinath, A.; Bhattacharjee, J.; Panda, T. K. *Chemical Communications*, **2019**, *55*, 1386-1389.
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Invited Lecture (IL-27)
International Conference on Organometallics and Catalysis (ICOC 2020)

C-H Bond Functionalization of Unactivated Arenes and Carbonyl Compounds via Scandium Catalysis

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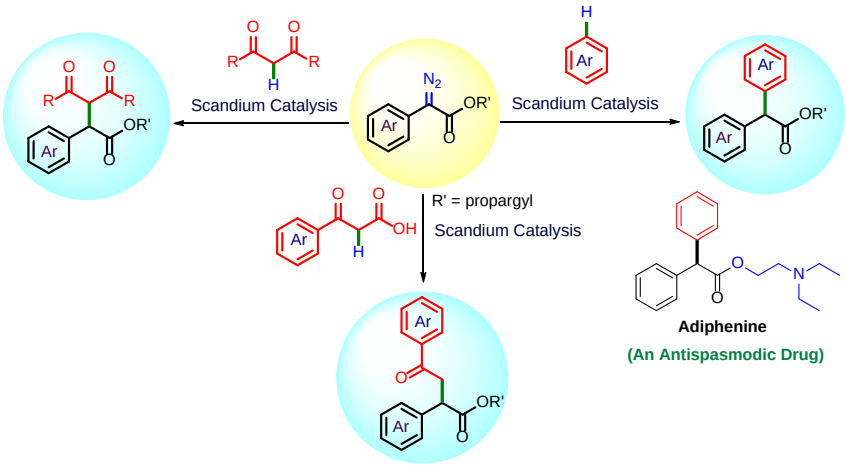
Abstract:
Catalytic C-H bond functionalization is one of the most important methods for the synthesis of complex organic molecules.[1] Developing catalytic methods for the chemo- and regioselective C-H bond functionalization is highly desirable but challenging task for the synthetic community. Substituted arenes are widespread in various biologically active compounds, and drug molecules.[2] As a part of our ongoing research programme, we have developed a robust propargyl α-aryl-α-diazoacetate as a new class of reagent for the effective C-H bond functionalization of unactivated arenes via scandium catalysis to access useful α-diarylacetates. Likewise, scandium catalysis has also been explored for the effective C(sp^3)-H bond functionalization of 1,3 diketones & β-keto acids along with propargyl α-aryl-α-diazoacetates. This presentation will provide an overview of some of the recent advancement in our laboratory on the C-H bond functionalization via scandium catalysis.



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Invited Lecture (IL-27)

International Conference on Organometallics and Catalysis (ICOC 2020)

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Ramakrishna G. Bhat (RGB) obtained his PhD in synthetic organic chemistry from the Department of Organic Chemistry, Indian Institute of Science (IISc) Bengaluru in 2004. He then moved to SFU, Vancouver, Canada for his postdoctoral research work. In the year 2006, he returned to India and started his independent career at IISER Pune and is currently serving as a Professor.

His research interests are in the area of Organic Synthesis and Catalysis. Currently, Prof. RGB's research group has been focussing on Organocatalysis, C-H functionalization and photoredox catalysis.

Development of Supramolecular catalytic ensembles for construction of C-C/C-X bond

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Abstract:

Our research work aims at development of supramolecular assemblies which served as nanoreactors for the preparation of metal NPs. During the reduction process, supramolecular assemblies undergo structural/chemical changes and in combination with metal/metal oxide NPs act as catalytic ensembles for carrying out various organic transformations in aqueous/mixed aqueous media. Recently, we have utilized same strategy for preparation of alloy metal NPs. We have developed hybrid Au-CuO NPs[1], Cu_2O-Fe_2O_3 NPs[2], $AgCu_2O$ NPs[3], Ag@Fe_3O_4 nanoclusters[4], Au-Fe_3O_4 nanodots[5,6] stabilized by supramolecular assemblies based on hexaphenylbenzene/pyrazine derivatives for carrying out Ullman Goldberg coupling, three component click reaction, preparation of indazole derivatives via C-C/C-N bond formation reactions.

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Invited Lecture (IL-28)

International Conference on Organometallics and Catalysis (ICOC 2020)

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Vandana Bhalla received her Ph.D from the Department of Chemistry, Guru Nanak Dev University She is presently working as Associate Professor at Department of Chemistry, Guru Nanak Dev University, Amritsar, India. Her current interest includes development of fluorescent probes and catalysis. She has published more than 185 research papers in international journals.

She has received various prestigious awards:

Bronze Medal awarded by Chemical Research Society of India (CRSI), Bangalore for the year 2015 for contributions in Chemical Sciences

Thomson Reuters Research Excellence India Citation Award 2015

Bhagya-Tara award by Panjab University for contribution in organic chemistry 2015

First Shiv Nath Rai Kohli Mid- Career Best Scientist Award for contribution in Chemical Sciences by Panjab University, Chandigarh 2018

Prof. S.S. Sandhu Endowment Award, 2017

Rajib Goyal Award by Kurukshetra University, KUK 2018.

Iminium-Activated Oxidant Free C-H Functionalization of Amines

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Abstract:
Iminium ions, which are traditionally formed via condensation of carbonyl compounds and amines, mediate large varieties of reactions. Most of these reactions functionalize the carbonyl component of the iminium ion in diverse ways such as, nucleophilic addition, isomerization-electrophilic addition, cycloaddition, etc.[1] However, the functionalization of the amine component of the iminium ion remains less explored.

The approach developed in our group for the selective functionalization of amine component of the iminium ion will be presented.[2] Direct carbo- or hetero-functionalization of alpha C-H or more challenging beta-C-H bonds of commercially available amines were achieved under operationally simple conditions without any aid of metal based reagent/catalyst and/or external oxidants. The C-H functionalization enabled multicomponent reactions (CH-MCRs) have been developed by altering the reactivity of classical multicomponent reactions (MCRs) through selective functionalization of the amine component. The reactions have the potential for practical application because of its operational simplicity and environmentally benign nature.

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Invited Lecture (IL-29)

International Conference on Organometallics and Catalysis (ICOC 2020)

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Chandan K. Jana received his M.S. in Chemical Science from the Indian Institute of Science Bangalore in 2005. In 2008, he received his Ph.D. from the University of Muenster, Germany, as a member of the International Graduate School of Chemistry. He then moved first to EPFL and then to the University of Basel, Switzerland, for his postdoctoral research (2009–2011). In 2011, he returned to India and started his independent research career as an Assistant Professor in the Department of Chemistry at the Indian Institute of Technology Guwahati, where he became Associate Professor in 2015 and Professor in 2019.

His research centers on synthetic organic chemistry, particularly, the development of new synthetic methodology and the synthesis of bioactive molecules and natural products.

Unusual Symmetric *bis*(C-H) Agostic Interactions in Linear Ni(I) complexes

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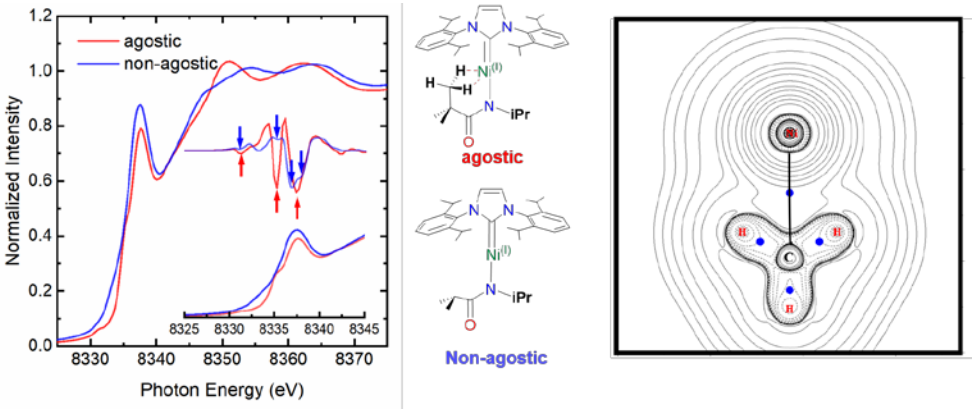
Abstract:
Agostic interactions play an important role in transition metal catalyzed C-H activation. These interactions are typically dominated by charge donation from the σ_{CH} bond into empty valence metal d orbitals.[1] Herein, we report an unusual bis(CH) agostic interaction in electron rich linear d9 Ni(I) complexes.[2,3] Ni K-edge X-ray absorption spectroscopy (XAS) show that the agostic interaction has a dramatic influence on the empty valence states with very little contribution from the valence metal d orbitals. Our experimental findings are supported by DFT results, which reveal an unconventional covalent agostic interaction with donation into the metal 4p orbitals with both σ and π charge donation from two mirroring C-H σ bonds into the 4p orbitals of the metal center. In this geometry, the bis(CH) ligand is best described as a σ and π donor leading to a surprisingly strong (50-80 kJ/mol) stabilization. The implications of this unusual bonding mode are discussed and contrasted with more typical agostic interactions.

Figure



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Invited Lecture (IL-30)

International Conference on Organometallics and Catalysis (ICOC 2020)

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Research Overview

My research centres on probing the relationship between ***electronic structure*** and ***reactivity*** in systems of importance in biological and chemical catalysis. Emphasis is placed on the application of element-specific spectroscopic techniques such as X-ray Absorption Spectroscopy (XAS) as a means of generating experimentally-validated electronic and geometric structure descriptions of catalytically relevant species. Our group is currently active in exploring the electronic structure of metal-dioxygen species, defining the role of ligand redox processes in the activation of late transition metal organometallic anticancer agents, probing the specific nature of sulfur-centered redox processes in biology, as well as exploring the role of transition metals as active biocidal agents

Some Aspect of Primary Amide Chemistry: Unexplored Directing Groups for C-H bonds Activation.

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Abstract:

Functionalized organic molecules are an important class of compounds that are ubiquitously present as a key structural motif in natural products, and biologically active compounds. The introduction of the required functional motif into the desired system with satisfying the parameters of sustainable chemistry such as cost and atom-economy are high in demands. Therefore, the direct activation/functionalization of robust and unreactive C-H (sp^2/sp^3) bonds provides an alternate, effective, and desirable tool to the organic chemists to convert them into the valuable chemical commodity.[1] However, major challenges lie with these methods regio- and chemoselectivity functionalization of C-H bonds. To overcome these issues, concept of directing group was introduced, where directing group act as a ligand and coordinate with metal-salt to form cyclo-metallated adducts and eventually offer chemoselective transformations.

Hence, in the past decade, a variety of directing groups such as acetanilides, pyridyls, oxazolyl, and N-substituted secondary and tertiary amides have been introduced for regioselective C-H transformation. In general, these strategies required the preinstallation of directing groups followed by their uninstallation, which demands two extra steps, resulting in the eventual reduction in the atom and step economy of the complete transformation. Despite the ubiquitous presence of primary amide (CH_2CONH_2), has been rarely utilized as a directing group owing to their least reactive nature and make an unattractive and challenging synthon. Considering the high abundance and challenge, we became interested in exploring the chemistry of primary amide as desired directing group for the synthesis of high value-added derivatives of organic compounds.[2] The scope and limitations of such chemistry will be discussed using selected examples.

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Invited Lecture (IL-31)

International Conference on Organometallics and Catalysis (ICOC 2020)

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Postdoctoral Fellow*:*

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- University of Konstanz, Germany: **2010-2012**

Employment:

- Research Investigator-Biocon-Bristol Myers Research Center, Bangalore: **2012- 2013**
- Assistant Professor, IIT Patna: **2014-4th Dec. 2019**
- Associate Professor, IIT Patna **5th Dec. 2019**

Publications from IITP: 20

AK research group primarily involves in the design and development of cost and atom-economical strategies for the syntheses of important functional organic molecules utilizing the chemistry of amides and imidates. Chemistry of ubiquitous amides and imidates functional groups has been well explored for the distal functionalization of robust C-H bonds of electronically complex molecules such as carbohydrates and aliphatic compounds. Indeed, our group also involves in the glycodiversification.

N-Heterocyclic Silylenes: Versatile Ligands in Homogeneous Catalysis

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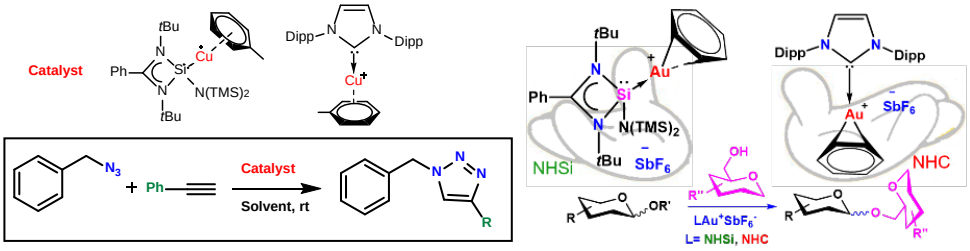
Abstract:
Development of new ligands to regulate the reactivity is of fundamental interest in transition metal catalysis. Of late, N-heterocyclic silylenes are emerging as a new class of steering ligands. Silylene transition metal complexes have been explored as catalysts for many important organic transformations and proven to be superior at several instances than classical ligands.[1] Usually, the transition metals involved in these reactions are Mn, Fe, Ni, Co, Rh, Ir, Pd, Pt etc. It is apparent that although silylenes have excelled in TM chemistry, they have surprisingly not been used as ligands in homogeneous catalysis mediated by the coinage metals (Cu, Ag, Au). Given our recent interests in silylene-coinage metal chemistry,[2] we have embarked into the silylene-Au(I)//Cu(I) complexes and utilized them as catalysts in click reaction,[3] C-N coupling reaction and polysaccharide synthesis.[4]

Figure 1: NHSi/NHC supported cationic Cu(I)- and Au(I)-arene complexes and their catalytic reactions.



References and Notes:

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4. Unpublished work.

Invited Lecture (IL-32)

International Conference on Organometallics and Catalysis (ICOC 2020)

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Shabana Khan obtained her PhD degree from the Indian Institute of Technology, Delhi in 2008. Subsequently, she received the fellowship of Deutscher Akademischer Austausch Dienst (DAAD) and joined the research group of Prof. Herbert W. Roesky as a postdoctoral fellow at University of Goettingen, followed by a second post doc with Prof. Manuel Alcarazo at the Max Planck Institute for Coal Research. Currently she is working as an associate professor in the Department of Chemistry, Indian Institute of Science Education and Research, Pune, India. Her research interest includes the synthesis of low-valent compounds, their reactivity and application in catalysis.

Invited Lecture (IL-33)
International Conference on Organometallics and Catalysis (ICOC 2020)

Electrochemical Synthesis of Biologically Relevant Heterocyclic Scaffolds

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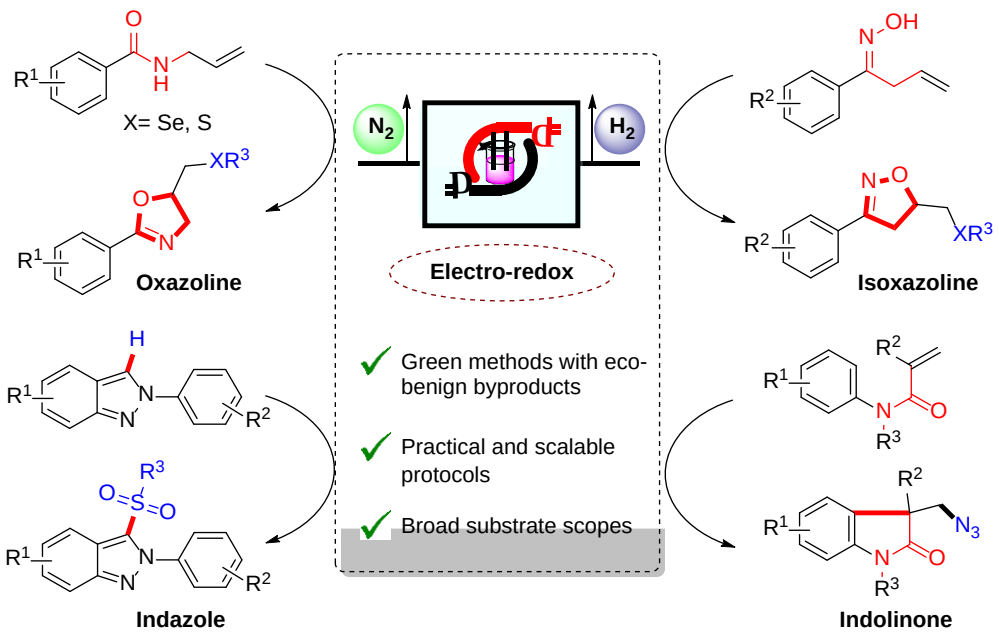
Abstract:
Electrochemistry is one of the most versatile and environmentally benign platforms for redox-mediated transformations in organic synthesis.[1] This electro-synthetic strategy is now globally accepted as a smart alternative for stoichiometric redox reagents and successfully excluding chemical wastes and toxic byproducts. In addition, the selectivity and efficacy of the redox processes can be controlled by fine-tuning of the current flow and applied potential.[2] Herein, we present the sustainable synthesis of several biologically relevant heterocyclic scaffolds under electrochemical conditions.[3] These external oxidants and metal-free green protocols reveal synthetic benefits in terms of easily accessible starting materials, short reaction times and also claim potential applications in large scale synthesis.



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3. De Sarkar, S. *Unpublished.*

Invited Lecture (IL-33)

International Conference on Organometallics and Catalysis (ICOC 2020)

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Suman De Sarkar obtained his Ph.D. in November 2010 from Westfälische Wilhelms University Muenster under the supervision of Prof. Armido Studer. Afterward, he worked as a postdoctoral researcher in the laboratories of Prof. Karl Gademann at the University of Basel and in the research group of Prof. Lutz Ackermann as an Alexander von Humboldt Postdoctoral Fellow at Georg-August-University, Goettingen. In October 2015 he joined Indian Institute of Science Education and Research Kolkata as an Assistant Professor and in September 2019 is been promoted to the post of Associate Professor. His main research interests focus on the development of Redox mediated transformations.

Synthesis and Reactivity of a Hypersilylsilylene

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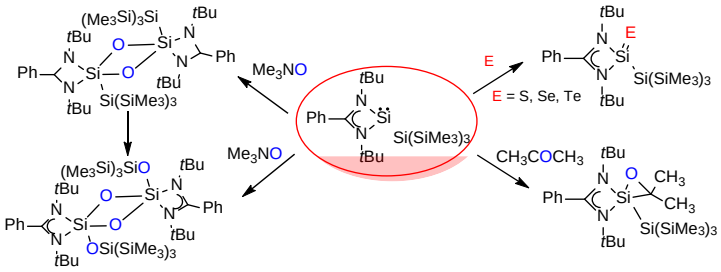
Abstract:
Since the pioneering work by Gilman and Smith on the synthesis of tetrakis(trimethylsilyl) silane,[1] there is an increasing use of the tris(trimethylsilyl)silyl group in the synthesis of numerous organometallic compounds. We have introduced this group in amidinate-silylene system through the isolation of an amidinate hypersilylsilylene, PhC(N*t*Bu)$_2$Si{Si(SiMe$_3$)$_3$}.[2] Subsequently, a series of reaction was performed with several small molecules which led to unprecedented product formation.[2,3] We will also show how the presence of the tris(trimethylsilyl)silyl group makes difference compared to other functionalized amidinato silylenes in product formation.

Figure 1: Reactions of a hypersilylsilylene



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After finishing his M.Sc. from IIT Kharagpur, India in 2006, Sakya S. Sen joined the research group of Prof. Herbert W. Roesky at the University of Göttingen, Germany and received the PhD degree in 2010 with summa kum laude (outstanding) grade. Then he joined as a postdoctoral researcher supported by the Alexander von Humboldt Foundation in the laboratory of Prof. Holger Braunschweig at the University of Würzburg, Germany. Since 2014, Dr. Sen is working in CSIR-National Chemical Laboratory, India as a senior scientist. Dr. Sen is the recipient of CSIR-Young scientist award in 2017, INSA medal for Young Scientist in 2018, Merck Young Scientist Award, 2019. He is a young associate of Indian Academy of Sciences (2017-2020). He has been selected as a ChemComm Emerging Investigator 2018, Inorganic Chemistry Emerging Investigator 2019, and Early Career Advisory Board Member of ACS Catalysis (2019-2021).

Organophosphites as Nucleophile Catalysis for Asymmetric Rearrangements and Radical Reactions

Abdul Motaleb, Siniya Rani, Asish Bera, Chandrakant Nichide, Pradip Maity*
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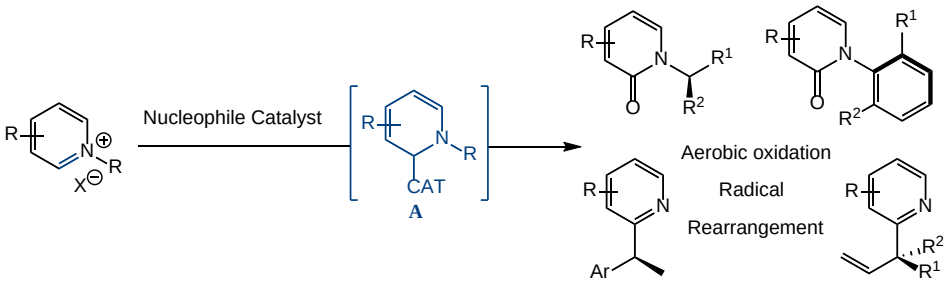
Abstract:
Molecular rearrangements have been one of the most frequently utilized synthetic methods and radical chemistry emerged as a fast-growing research field in recent times. Unfortunately, stereoselective transformations for both of these approaches are scarce.[1,2] Our interest in regio- and stereoselective C–H functionalization of feedstock azaarenes to value-added products prompted us to take advantage of the embedded imine in them. We will present our development of a nucleophile catalysis platform to tackle the problem with economic and environmental benefits.



Scheme: Catalyst controlled aerobic oxidation and molecular rearrangements.

Six-membered N-heteroaromatics (azaarenes) and five-membered double-heteroaromatics with embedded imine polarize the π-system and can be regarded as "carbonyl equivalent." The N-quarterization increases its electrophilicity, and a nucleophilic catalyst can form the corresponding adduct (**A**). We are exploring the reactivity of this adduct for various radical and rearrangement reactions. We will present aerobic auto-oxidation protocol; with catalyst control oxidative kinetic resolution having an α-stereogenic center to nitrogen.[3] The adduct **A** has also been utilized for anionic aza-Wittig rearrangements where rearomatization via catalyst release drives the energetically unfavorable aza-rearrangements. The N-allyl salt undergoes asymmetric allylic alkylation with chiral TADDOL based phosphites with broad substrate scope.[5] We will also discuss our experiences with different competitive rearrangement[4] and other reaction types; and our efforts to override the inherent substrate control preference to obtain a product of our choice.

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Invited Lecture (IL-35)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Senior Scientist

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Group Homepage: http://academic.ncl.res.in/p.maity

Research Interest

New asymmetric synthetic methodology in the broad area of radicals and molecular rearrangements; Sustainable catalysis; Economic process development for APIs

Education and Appointments

- **March 2015 – Present**: Senior Scientist, Organic Chemistry Division, CSIR-National Chemical Laboratory, Pune
- **September 2011 – February 2015**: Postdoctoral Researcher, UT Southwestern Medical Center
  Mentor: Prof Uttam K. Tambar
- **January 2006 – August 2011:** Ph.D. in Synthetic Organic Chemistry, Florida Atlantic University
  Mentor: Prof Salvatore D. Lepore
- **May 2001 – May 2003:** MSc in Chemistry, Indian Institute of Technology, Kanpur, India
  Mentor: Prof Faiz A. Khan
- **March 1998 –March 2003:** BSc in Chemistry (Hons), Ramakrishna Mission Residential College, Narendrapur; Calcutta University, India

Research Experience

- **Postdoctoral research:** Organocatalytic [2,3] and [3,3] rearrangements • [3,3] aza-Claisen rearrangement • Vinylogous Pictet-Spengler cyclization • Indole and indolinone containing bioactive and natural products of pharmaceutical interest

- **Ph.D. research:** Synthesis of functionalized allenyl and alkynyl carbonyls from 1,3-dicarbonyls • Functionalization of γ-silylallenyl esters to γ-carbinolallenoates • Ammonium ion catalyzed cyclization of β-alkynylhydrazines to chiral azaprolines via kinetic resolution • Synthesis of fully functionalized core structure of a congested bridged bicyclic diketo compound, vitisinol D (anti-thrombotic natural product) and vitisinol C

Invited Lecture (IL-36)

International Conference on Organometallics and Catalysis (ICOC 2020)

Enzyme-inspired designing of synthetic hydrogen production catalysts

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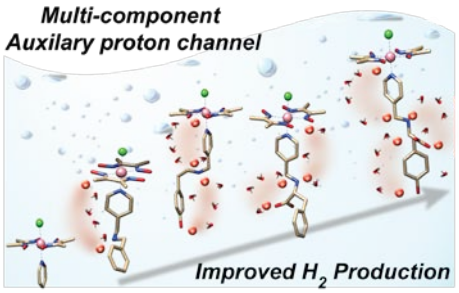
Abstract:
A swift transformation of solar energy into the H-H chemical bond (in H_2 molecule) is one of the crucial steps for the implementation of H_2-based renewable energy infrastructure. The search for a perfect model of H_2 producing catalyst for this purpose is still on due to the intrinsic shortcomings of platinum-based materials and natural hydrogenase enzyme. Here, in this work, we have included the hallmarks of both synthetic catalyst and enzymatic architecture during the design of cobalt-based H_2 producing molecular catalysts. We have developed a canopy of basic functionalities around a synthetic cobalt complex core emulating the protein-based outer coordination sphere (OCS) in enzymes. Incorporation of this model OCS feature enabled us to develop a new genre of purely water-soluble, oxygen tolerant, and H_2 producing cobaloxime complexes. The peripheral functionalities directly influenced the proton movement around the cobalt core to significantly improve electro- and photocatalytic H_2 production in aqueous media. Interestingly, these cobalt complexes exhibited excellent photocatalytic H_2 production in the presence of organic dye, Eosin-Y, even under natural sunlight in neutral, aerated aqueous medium (pH 7.0).[1] Hence, the rational design of synthetic catalyst containing enzymatic features has allowed us to develop practical condition ready synthetic catalysts for H_2 production.

Figure:



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Invited Lecture (IL-36)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Arnab started his career in Chemistry with B.Sc. from Presidency College, Kolkata in 2002. He joined IIT Bombay for his M.Sc. in 2005. Arnab got his PhD from Arizona State University in 2012 before moving to Pacific Northwest national Laboratory. Arnab Joined IIT Gandhinagar as an assistant Professor in 2015. His research interest lies in developing enzyme-inspired molecular catalyst for renewable energy relevant chemical transformations.

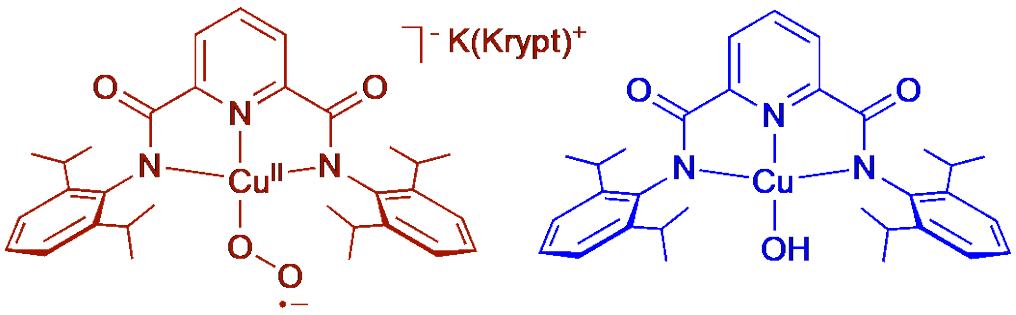
Invited Lecture (IL-37)
International Conference on Organometallics and Catalysis(ICOC 2020)

Proton-Coupled Electron Transfer Mechanisms in Copper-Oxygen Chemistry

William B. Tolman

*Department of Chemistry, University of Minnesota, Minneapolis, MN. *Current address: Department of Chemistry, Washington University in St. Louis, St. Louis, MO.*
(E-mail: wbtolman@wustl.edu)

Abstract:
Characterization of copper intermediates in enzymes and other catalysts that attack strong C-H bonds is important for unraveling oxidation catalysis mechanisms and, ultimately, designing new, more efficient catalytic systems. New insights into the nature of such intermediates may be obtained through the design, synthesis, and characterization of copper-oxygen complexes. Particular impetus for such studies comes from provocative proposals of novel structures for the oxidizing species a variety of monocopper enzymes, of which lytic polysaccharide monooxygenase (LPMO) is of particular note due to its novel structure and its utility in biotechnology. In work aimed at synthesizing molecules with such cores, we have turned to the use of strongly electron donating carboxamide ligands designed to stabilize copper in high oxidation states. In this lecture, we focus on comparing the reactivity of complexes with [CuO2]+ and [CuOH]2+ cores having the same supporting ligand with C-H and O-H bonds. Intriguing differences in their mechanisms of proton-coupled electron-transfer will be discussed.



Bio-Sketch of speaker

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William B. Tolman is an inorganic chemist whose laboratory works on synthesis and characterization of bioinorganic systems, organometallic reagents and polymers. He received his bachelor's degree in Chemistry from Wesleyan University in 1983, and then completed a Ph. D. He completed postdoctoral study from Massachusetts Institute of Technology from 1987 to 1990 with Prof. Stephen J. Lippard. Current research in his group emphasizes the use of synthetic chemistry to unravel how copper-containing enzymes function and developing new ways to prepare biorenewable and sustainable polymers. His team has published more than 200 papers in peer-reviewed journals, and he is a fellow of both the American Chemical Society and the American Association for the Advancement of Science. He is also editor-in-chief of the American Chemical Society Journal Inorganic Chemistry.

Before coming to Washington University in January 2018, Tolman spent 27 years at the University of Minnesota, where he was the Distinguished McKnight University Professor and chair of the Department of Chemistry (2009-2017).

Selected Awards / Honors:

American Chemical Society Award for Distinguished Service in the Advancement of Inorganic Chemistry, 2017

Charles E. Bowers Teaching Award (College of Science & Engineering, University of Minnesota), 2012

Fellow of the American Chemical Society, 2010

Fellow of the American Association for the Advancement of Science, 2006

Alexander von Humboldt Foundation Research Award at TU Munich, 2004

Research Award, Alexander von Humboldt Foundation, 2004

Buck-Whitney Medal (American Chemical Society, Eastern New York Section), 2001

Distinguished McKnight University Professorship (University of Minnesota), 2000

George W. Taylor Award for Excellence in Research (University of Minnesota), 1998

Camille & Henry Dreyfus Teacher-Scholar Award, 1994-1999

National Young Investigator Award (National Science Foundation), 1993-1998

Bush Sabbatical Supplement Award (University of Minnesota), 9/96-6/97

Invited Lecture (IL-38)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

Dr. Milton "Mitch" R. Smith

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Milton "Mitch" R. Smith, III was born in El Paso, Texas, and spent his childhood in Texas, Iowa, and West Virginia. He received his B.S. degree in 1986 from Caltech, where he carried out research with Professor Terrence. J. Collins. After graduation, Mitch spent the summer as a research intern at Monsanto, Co. before beginning his graduate studies under the tutelage of Professor Gregory L. Hillhouse at the University of Chicago. At Chicago, his thesis work centered on the synthesis and reactivity of metal diazene complexes. After receiving his Ph. D. in 1990, he was awarded a Miller Fellowship at the University of California, Berkeley, where he spent two years synthesizing and exploring the reactivity of early transition metal oxo and imido complexes in the laboratories of Professor Richard A. Anderson. In 1992, Smith began his independent career and Michigan State University as an Assistant Professor in the Chemistry Department. There he built began a research program centered on the reactivity of transition metal complexes with organoboron reagents. He was promoted to Associate Professor with tenure in 1997 and Full Professor in 2002.

In 1999, Professor Smith and his graduate student, Carl Iverson, reported a thermal, catalytic synthesis of an organoborane from a borane and a hydrocarbon where the sole byproduct was hydrogen gas. This landmark in C–H bond functionalization led to a family of highly efficient iridium catalysts that operate on a wide variety of aromatic and heteroaromatic compounds. Smith co-founded BoroPharm, Inc. with MSU colleague Professor Robert E. Maleczka, Jr. and CEO Todd Zahn. In 2008, Smith was a co-recipient of an award from the Presidential Green Chemistry Challenge Award for his contributions to C–H functionalization. In addition to C–H functionalization, Smith's research interests include polymer nanomaterials and energy storage and conversion.

Invited Lecture (IL-39)
International Conference on Organometallics and Catalysis (ICOC 2020)

On discovery in catalysis

Frank Glorius*
Department of Chemistry & Pharmacy
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Abstract:
Catalysis is a key technology of our modern societies, since it allows for increased levels of selectivity and efficacy of chemical transformations. While significant progress can be made by rational design or engineered step-by-step improvements, many pressing challenges in the field require the discovery of new and formerly unexpected results (**Figure 1**). Arguably, the question "How to discover?" is at the heart of the scientific process. In this talk, strategies and discoveries from the Glorius group will be discussed. Topics will include the use of N-heterocyclic carbenes (NHCs)[1] in different fields of catalysis (such as arene hydrogenation[2] and on-surface chemistry[3]) and also discovery and reproducibility in photocatalysis.[4-6]

Figure: "Landing of Columbus at the Island of Guanahani, West Indies, 12 October 1492", John Vanderlyn, 1836-47

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5. M. Teders, C. Henkel, L. Anhäuser, F. Strieth-Kalthoff, A. Goméz-Suárez, R. Kleinmans, A. Kahnt, A. Rentmeister, D. M. Guldi, F. Glorius, *Nat. Chem.* **2018**, *10*, 981.
6. L. Pitzer, F. Schäfers, F. Glorius, *Angew. Chem. Int. Ed.* **2019**, *58*, 8572.

Invited Lecture (IL-39)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Professor

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University of Muenster
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Frank's research program focusses on the development of new concepts for diverse areas of catalysis such as photocatalysis, C–H activation, smart screening and data-based technologies including machine learning, N-heterocyclic carbenes (NHCs) in organocatalysis and as surface modifiers and in (asymmetric) arene hydrogenation. He is also interested in modern batteries and the manipulation of membranes. He published more than 300 independent papers (peer reviewed), was cited more than 32.000 times and has an H-index of 95. His work was highlighted with several awards such as the German Leibniz Award, the American ACS Cope Scholar Award, the Japanese Mukaiyama Award or the international OMCOS Award. He is most proud on the large number of excellent group members, who moved on and who have become leaders in industry and academia themselves.

Academic Career

Since 08/2007	**Münster:** Full Professor of Organic Chemistry at the WWU Münster
2004 - 2007	**Marburg:** C3-Professor for Chemistry at the University of Marburg
2001 – 2004	**MPI:** Independent research at the MPI für Kohlenforschung (**Fürstner**)
2000 - 2001	**Harvard:** Postdoctoral studies at Harvard University (**Evans**)
1997 - 2000	**Basel&MPI:** PhD at University of Basel & MPI für Kohlenf. (**Pfaltz**)
1996 - 1997	**MPI&Hannover:** Diploma thesis at MPI (**Pfaltz/Hoffmann**)
1995 - 1996	**Stanford:** Research studies at Stanford University (**Wender**)
1992 - 1997	**Hannover:** Studies of chemistry at the University of Hannover

Invited Lecture (IL-40)
International Conference on Organometallics and Catalysis (ICOC 2020)

New Arylation Strategies for Organic Synthesis

Michael Greaney*
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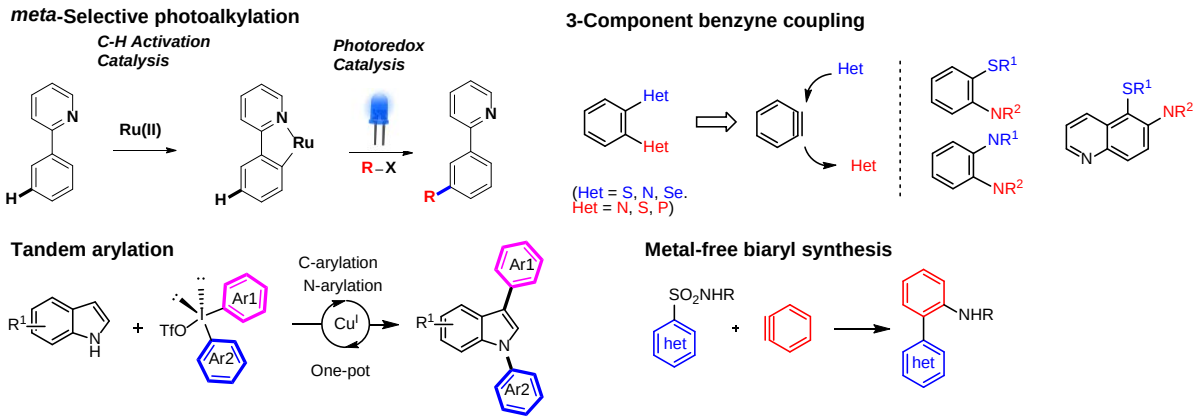
Abstract:
Transition metal (TM) catalysts can control a vast range of chemical reactivity. At one extreme, they can harness and modulate the most energetic reactive intermediates, such as arynes and carbenes. Contrastingly, they can be used to activate inert, unreactive functional groups such as C-H bonds. Both of these areas offer tremendous potential for the discovery of new, catalytic reaction pathways for C-C and C-X bond construction. Focussing on the heterocyclic field, the talk will describe our progress in designing new TM-catalysed reaction systems and their application to modular heterocycle synthesis. [1,2]



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1. C. M. Holden, S. A. M. Sohel, M. F. Greaney, *Angew. Chem. Int. Ed.* **2016**, *55*, 2450-2453. J. A. Garcia-Lopez, M. Cetin, M. F. Greaney, *Angew. Chem. Int. Ed.* **2015**, *54*, 2156-2159.

2. S. G. Modha, M. F. Greaney, *J. Am. Chem. Soc.* **2015**, *137*, 1416-1419. C. J. Teskey, S. M. A. Sohel, D. Bunting, S. Modha, M. F. Greaney, **2017**, *56*, 5263–5266

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Invited Lecture (IL-40)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

Dr. Michael Greaney
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School of Chemistry
University of Manchester
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Homepage: https://www.research.manchester.ac.uk/portal/michael.greaney.html

Michael Greaney took his undergraduate degree at Oxford, completing his part II research project in the group of Sir Jack Baldwin, followed by PhD work with William Motherwell at UCL, completing his thesis in the area of new fluorinating agents in 1999. He then left the UK on a GlaxoWellcome scholarship to take up a postdoctoral position with Jeffrey Winkler at the University of Pennsylvania, where he worked on the total synthesis of the tumour-promoting diterpene ingenol. He returned to the UK in early 2002, to a lectureship position at the University of Edinburgh. He was awarded an EPSRC Leadership Fellowship in 2008, and in 2011 moved to the University of Manchester to a personal chair in organic chemistry. His research interests cover transition-metal catalysed C-H activation, photochemistry, aryne chemistry, tandem reactions, and reversible reactions for dynamic covalent chemistry.

He is the recipient of the 2011 SCI Syngenta, Pfizer, Astrazeneca award for process chemistry research, and the 2017 RSC Bader award in organic chemistry.

Borametallomimetics – Activation of Small Molecules by Low-valent Boron Species

Holger Braunschweig
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Abstract:

The activation of small molecules is generally associated with transition metals (TM) and constitutes the basis of catalysis. It was believed that TM catalysts are required to facilitate processes such as the activation of H_2 and other unreactive substrates. However, recent years have witnessed exciting developments in main group element chemistry, and the discovery of carbenes, FLPs and heavy main group species that are capable of TM-like activation reactions.[1]

Our ongoing studies on borylenes, diborenes, and diborynes have shown that these low-valent species exhibit a very rich chemistry, which is distinctly different from that of common compounds deriving from boron in oxidation state +3. Particularly interesting is the metal-like behavior of some borylenes and diborynes, which form CO complexes analogous to TMs, bind H_2 and unsaturated organic substrates under mild conditions and even activate N_2.[2]

References

[1a] P. P. Power, *Nature*, **2010**, *463*, 171; [b] G. C. Welch, R. R. San Juan, J. D. Masuda, D. W. Stephan, *Science*, **2006**, *314*, 1124; [c] G. D. Frey, B. Lavallo, B. Donnadieu, W. W. Schoeller, G. Bertrand, *Science*, **2007**, *316*, 439.
[2a] H. Braunschweig, R. D. Dewhurst, F. Hupp, M. Nutz, K. Radacki, C. Tate, A. Vargas, Q. Ye, *Nature*, **2015**, 327; [b] H. Braunschweig, K. Radacki, A. Schneider, *Science*, **2010**, *328*, 345; [c] H. Braunschweig, R. D. Dewhurst, K. Hammond, J. Mies, A. Vargas, K. Radacki, *Science*, **2012**, *336*, 1420; [d] M.-A. Légaré, G. Bélanger-Chabot, R. D. Dewhurst, E. Welz, I. Krummenacher, B. Engels, H. Braunschweig, *Science*, **2018**, *359*, 896.

Invited Lecture (IL-41)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Education

1988	Diploma in Chemistry, RWTH Aachen
1990	Dr. rer. nat., RWTH Aachen, Germany (Prof. P. Paetzold)
1998	Dr. Habil., RWTH Aachen, Germany (Prof. P. Paetzold)

Professional Career

1991-1992	Postdoctoral researcher, University of Sussex, UK (Prof. M. F. Lappert, FRS)
1998	Privatdozent, RWTH Aachen
2000	Senior Lecturer in Chemistry, Imperial College, London, UK
2002	Reader in Chemistry, Imperial College, London, UK
2002-2009	Professor (C4) of Inorganic Chemistry, Univ. Würzburg, Germany
2005-2009	Dean and Vice-Dean, Fakultät für Chemie und Pharmazie, Univ. Würzburg
2009-	Professor (W3) of Inorganic Chemistry, Univ. Würzburg
2010	Chair at Friedrich-Alexander-Universität Erlangen-Nürnberg (declined)
2012-	Head of Inorganic Chemistry, Univ. Würzburg

Awards and Honors

Gottfried Wilhelm Leibniz Prize of the DFG (2009); Member of the Bavarian Academy of Sciences (2009); ERC Advanced Grant (2011); Member of the Leopoldina - German National Academy of Science (2011); Steinhofer Lecture, Universität Freiburg (2012); Bruker Lecture, University of Toronto (2014); ScotCHEM Invited Lectureship from the five Scottish universities (2014); RSC Main Group Award, Royal Society of Chemistry (2014); ERC Advanced Grant (2015); Corresponding Member of the North Rhine-Westphalian Academy of Sciences, Humanities and the Arts (2015); Frontiers Visiting Lectureship, Texas A&M University (2016); Alfred Stock Memorial Prize of the GDCh (2016); Glenn Seaborg Lecture, University of California Berkeley (2017); Leibniz Lecture Tour, Universities of Calgary and Ottawa, Canada (2017); Reinhart Koselleck Grant of the DFG (2018); JSPS Invitational Fellowship / Lecture Tour (2018)

Invited Lecture (IL-42)
International Conference on Organometallics and Catalysis (ICOC 2020)

Pnictinidenide Adducts of N-Heterocyclic Carbenes

Matthias Tamm*
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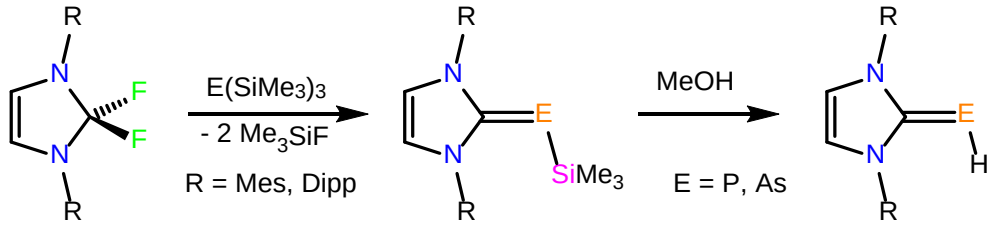
Abstract:
Soon after the advent of stable N-heterocyclic carbenes (NHC),[1] pnictinidene adducts such as (NHC)ER (E = P, As; R = Ph, CF_3, C_6F_5) were among the first carbene complexes of p-block elements to be prepared directly from free carbenes and suitable main-group compounds.[2] Our group has contributed to this field by preparation of NHC-supported phosphinidenes and arsinidenes (NHC)ER (E = P, As; R = $SiMe_3$, H) through reaction of 2,2-difluoroimidazolines (NHC)F_2 (NHC = IDipp, IMes) with E($SiMe_3$)$_3$ (E = P, As; Scheme 1).[3,4] These complexes were used for the preparation of transition metal complexes of the type [(NHC)EML_n][3,5] and for the preparation of heteroleptic dicarbene-dielement species of the type[(NHC)EE'(NHC)] (E, E' = P, As).[6–8] Along these lines, recent applications of the novel (NHC)E-transfer reagents in transition metal and main-group element chemistry and potential applications in homogeneous catalysis will be discussed.[9]



Scheme: Preparation of NHC-pnictinidene adducts.

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Invited Lecture (IL-42)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Matthias Tamm was born in Berlin, Germany, in 1967 and studied chemistry at the Technische Universität Berlin, where he received his PhD in 1992 under the supervision of F. Ekkehardt Hahn. After spending one year as a Visiting Research Scientist at DuPont Central Research and Development, DE, USA with Anthony J. Arduengo, III, he returned to Germany in 1994 to complete his Habilitation in Berlin and Münster. Tamm was appointed to Privatdozent at the Westfälische Wilhelms-Universität Münster in 1999 and held a temporary professorship at the Technische Universität München from 2002 to 2005. He then moved to the Technische Universität Braunschweig in 2005 to become Full Professor of Inorganic Chemistry. At this institution, he served as Dean of Studies (2009–2011) and as Dean of the Faculty of Life Sciences (2015–2017) and is currently acting as head of the Institute of Inorganic and Analytical Chemistry and as an elected member of the Senate of TU Braunschweig. He received honorary doctorates from the University Politehnica of Bucharest and from the Alexandru Ioan Cuza University Iași and in 2016 the Gheorghe Spacu Medal of the Romanian Chemical Society. His research interests lie in the areas of preparative organometallic chemistry and coordination chemistry with an emphasis on the development of novel, unusual ligand systems and on the application of their transition metal complexes in homogeneous catalysis, organic synthesis and materials science.

Invited Lecture (IL-43)
International Conference on Organometallics and Catalysis (ICOC 2020)

Synthesis of Metallosupramolecular Assemblies from Poly-N-Heterocyclic Carbene (poly-NHC) Ligands and their Postsynthetic Modification

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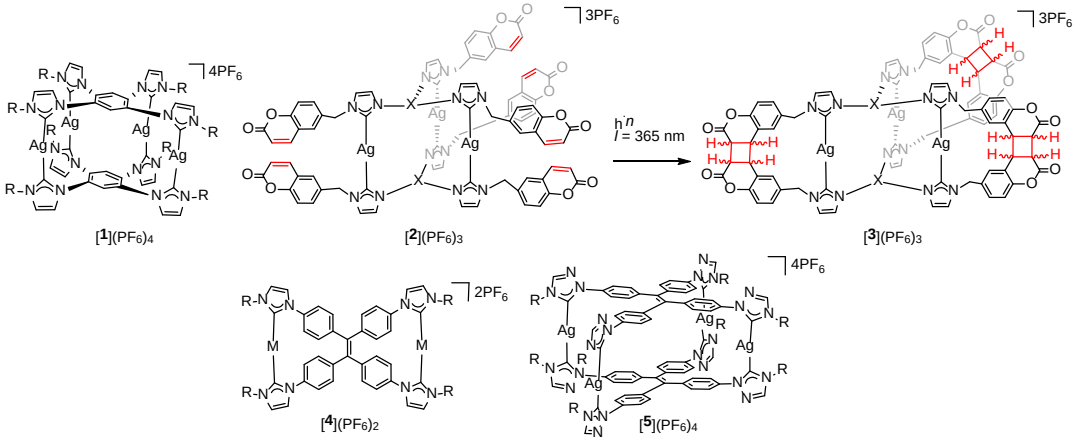
Abstract:
Three-dimensional, cylinder-like metallosupramolecular assemblies like [**1**](PF$_6$)$_4$ have been obtained from 1,2,4,5-tetrakisimidazolium substituted benzene and silver oxide.[1] Similarly, trinuclear cylinder-like assemblies [**2**](PF$_6$)$_3$ were obtained from 1,3,5-trisimidazolium substituted benzene[2] and Ag$_2$O. Narcissistic self-sorting was observed during the preparation of these assemblies.[3,4] Substitution of the trinuclear assemblies of type [**2**](PF$_6$)$_3$ with terminal N-olefins allows for a triple [2+2] cycloaddition involving pairs of olefins leading to trinuclear complexes [**3**](PF$_6$)$_3$ bearing a cage-like, tricyclic hexakis-NHC ligand. Removal of the metal ions yields tricyclic hexakisimidazolium cages.[5] The extension of this concept to dodecakis- and octadecakisimidazolium cages has been demonstrated.[6] Tetrakisimidazolium-substitutet tetraphenylethylene (TPE) reacts with Ag$_2$O to give the dinuclear complex [**4**](PF$_6$)$_2$ which exhibits luminescence due to rigidification by complex formation (as an alternative to AIE).[7] Use of 1,2,4-triazolium substituted TPE leads to tetranuclear (such as [**5**](PF$_6$)$_4$) or octanuclear luminescent assemblies.[8] This subject has been reviewed.[9]



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Bio-Sketch of Speaker

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FEH received his doctoral degree from the Technische Universität Berlin in 1985 under the supervision of the late Professor H. Schumann. After a postdoctoral stay at the University of California, Berkeley (1985–1988), working with Professor K. N. Raymond, he returned to the Technische Universität Berlin, where he completed the Habilitation in 1991. He moved to the Freie Universität Berlin as an Associate Professor of Chemistry in 1993. In 1998 he moved to his current positon as Full Professor of Inorganic Chemistry at the Westfälische Wilhelms-Universität Münster. He has been a visiting professor at the University of California Berkeley (1993), the National University of Singapore (2002), the University of Auckland (2009), Taiwan National University (2011), the University of the Negev, Israel (2012), the Univerity of Tasmania, New Zealand (2015) and the Federal University of Minas Gerais, Belo Horizonte, Brasilia (2019). He has been a Concurrent Professor at Fudan University, Shanghai (2015–2018) and he currently holds the position of Concurrent Professor at Nothwest University Xi'an, China.

Bioinspired Approaches to Selective Catalytic Oxidations by Nonheme Iron Complexes

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Abstract:
Dioxygen activating nonheme iron enzymes catalyze a myriad of biological oxidations such as hydroxylation of aliphatic C-H bonds, *cis*-dihydroxylation/epoxidation of alkenes, C-H halogenations etc.[1] High-valent metal-oxo intermediates, capable of transferring oxygen atoms into the C–H and C=C bonds of substrates, have been implicated as the active oxidants in enzymatic reactions. Inspired by the diverse biological oxidations by nonheme enzymes, several synthetic iron catalysts have been developed.[2,3] However, the selective electron transfer for the reductive activation of dioxygen without quenching the active species remains a major issue in performing bio-inspired oxidation catalysis with dioxygen by iron-based catalyst. Hence, most of the bio-inspired catalysts developed so far had to shunt this reduction process with peroxides or other oxidants.[3] But most of the catalytic systems often exhibit non-selective oxidation of substrates due to the involvement of free radicals generated in the catalytic conditions.

To address these challenges, we have been exploring different strategies toward catalyst design. The desired properties for iron catalysts are possible to achieve by using sacrificial reductants coordinated to the metal center for controlled reduction of dioxygen.[5a-c] In case of peroxide activation, the generation of metal-based oxidant through heterolytic O-O bond cleavage of iron(III)-OOH(R) may be tuned (i) by using Lewis/protic acid, (ii) by taking the advantage of secondary coordination interactions or (iii) by immobilizing iron complexes on solid surface.[4] In that direction, we have developed several bioinspired iron complexes of nitrogen rich ligands that activate dioxygen/peroxides leading to the generation of iron-oxygen oxidants.[5a-c] The active oxidants thus generated exhibit versatile reactivity including *cis*-dihydroxylation/epoxidation of alkenes and aliphatic C-H bond hydroxylation. The role of Lewis/protic acid and secondary interactions/surface immobilization on the reactivity of iron(III)-OOH(R) species have been evaluated.[5d-f] The reactivity of the dioxygen/peroxide-derived iron-oxygen oxidants and the ability of the complexes in performing selective catalytic oxidations will be presented in the talk.

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Invited Lecture (IL-44)

International Conference on Organometallics and Catalysis(ICOC 2020)

Bio-Sketch of Speaker

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Tapan Kanti Paine obtained the M.Sc. (Chemistry) in 1998 from the Indian Institute of Technology, Kharagpur. He carried out his graduate studies at the Max Planck Institute for Bioinorganic Chemistry, Germany during 1999-2002. After his Ph.D. in 2003, he moved to the University of Minnesota, USA to carry out postdoctoral research. In 2006, he returned to India to join the Indian Association for the Cultivation of Science, Kolkata, where he is currently a Professor in the School of Chemical Sciences. His area of research includes biomimetic inorganic chemistry, bioinspired catalysis, and mechanistic studies of O_2-dependent oxidative transformations.

Invited Lecture (IL-45)
International Conference on Organometallics and Catalysis (ICOC 2020)

Homo- and Hetero-Tetrasubstituted Double Bonds by Pd Catalysis

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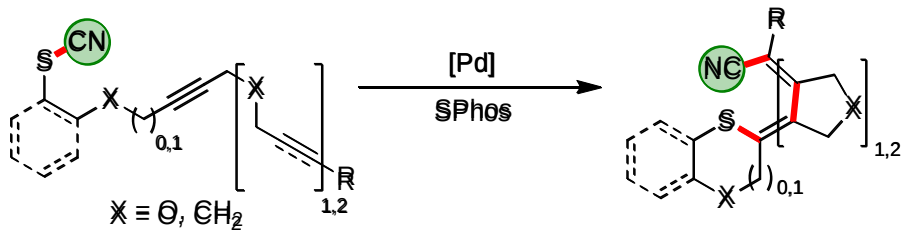
Abstract:
An important method of accessing tetrasubstituted double bonds is the dual functionalization of internal alkynes.[1] In its ideal and atom-economic way a substrate X-Y is attached to the C-C triple bond in a completely regio- and diastereoselective fashion. Depending on the type of substituents, either specially designed reagents are required or transition-metal catalysts are employed.

Some years ago, we designed an *anti*-carbopalladation reaction to C-C triple bonds that leads to two new single bonds across the emerging double bond.[2] While originally two carbon substituents were attached,[2,3] we extended the transformation to the substitution with oxygen and nitrogen substituents leading to the formation of highly substituted enol ethers and enamines.[4]

Recently, we employed – in lieu of an initial carbopalladation step a thiopalladation step leading to sulfur-substituted double bonds. When thiocyanates and several alkyne moieties are subjected to the transformation, a casacade takes place resulting in diene and triene systems with translocation of the cyano group.[5]



Scheme 1: Cascade consisting of thiopalladation, carbopallation, and cyanide transfer

References and Notes:

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Daniel B. Werz received a BS in chemistry at Heidelberg University, Germany, in 1997 and a Ph.D. in organic chemistry from Heidelberg University in 2003 with Rolf Gleiter. Following his doctoral studies, he was a Postdoctoral Fellow with Peter H. Seeberger at ETH Zurich, Switzerland. In December 2006 he joined the Chemistry Faculty of Göttingen University as an Assistant Professor of Chemistry under the mentorship of Lutz F. Tietze. In 2013 he took the position of an Associate Professor at the University of Braunschweig, in 2018 he was promoted at the same university to full professor. His main research interests include the development of novel efficient methods for the synthesis of hetero- and carbocyclic compounds (e.g. by cyclopropane chemistry, domino reactions and Pd catalysis). In addition, he is interested in carbohydrates and fluorescent dyes.

His awards include *inter alia* an Emmy Noether Fellowship of the German Research Foundation, a Heisenberg Fellowship, the ORCHEM Award, a JSPS Visiting Professorship in Japan, and an ERC Consolidator Grant. In 2017 he received a guest professorship at the IIT Bombay, in 2018 he has become visiting scholar at Tel Aviv University in Israel.

Invited Lecture (IL-46)
International Conference on Organometallics and Catalysis (ICOC 2020)

Activation of E-H bonds (E = B, C or Si) using Ru-borate complexes

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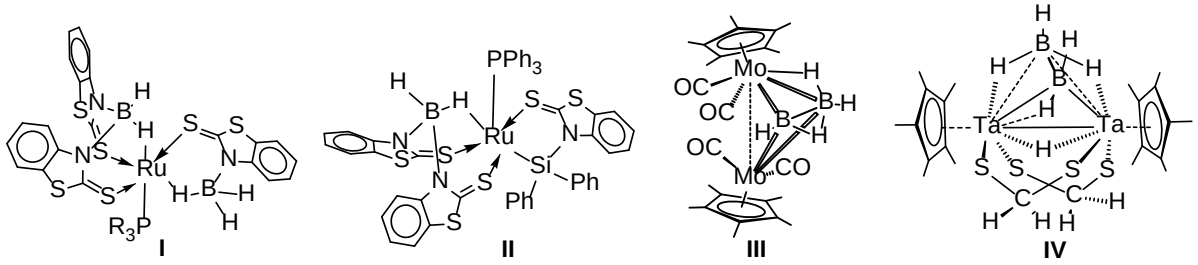
Abstract:
Over the few decades, there has been a significant interest in cooperation between metals and semimetal species (boron, silicon etc.) in mediating chemical reactivity. For example, boranes or silane can be captured or split by Lewis base at the metal centres and this approach has been adopted in various catalytic processes such as hydroboration, hydrosilylation and hydrogenation.[1] During these catalytic processes, [M]···H-B agostic or σ-complexes are generated as intermediate through metal-assisted B-H bond activation.[2] In this context, we have synthesised a series of 1,3-*N*, S-chelated Ru borate complexes which are capable of activating E-H bonds (E = B, C or Si) (**I** and **II**). On the other hand, diboranes and their derivatives are also of considerable importance due to their application in many organic syntheses, for example, hydroboration, diboration or borylation reactions. As a result, the structures of different diborane species are continuously studied for the complete understanding of their bonding. In this connection, we have isolated and structurally characterized various transition metal diborane complexes (**III** and **IV**).[3] The key results will be presented.



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Invited Lecture (IL-46)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Biography:

Prof. Sundargopal Ghosh obtained his B.Sc. and M.Sc. from University of Calcutta. He then received his PhD from Indian Institute of Technology Bombay in 1998. Following a postdoctoral fellowship with Professor Thomas P. Fehlner at the University of Notre Dame, USA he joined the Department of Chemistry at Indian Institute of Technology Madras in 2005 where he is currently a Professor. His research interests lie in the area of transition metal-boron compounds and their application in catalysis and small molecule activation. He has over 200 scientific publications in internationally acclaimed journals. For his contribution in chemical science, Chemical Research Society of India (CRSI) in 2013 conferred him with Bronze Medal and he was awarded Institute Research & Development Awards (IRDA) in 2014 by IIT Madras. He is an elected fellow of Indian Academy of Sciences (FASc) and Fellow of the National Academy of Sciences (FNASc). He is awarded Professor Priyadaranjan Ray Memorial Award in 2019. He has supervised 20 PhD students; most of them hold positions in well-known academic institutions.

Invited Lecture (IL-47)

International Conference on Organometallics and Catalysis (ICOC 2020)

Total Synthesis Driven Methodologies

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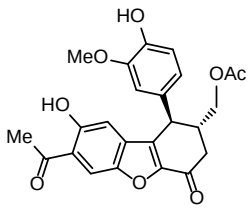
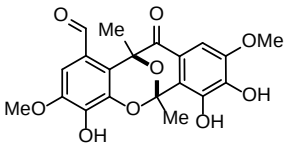
Abstract:

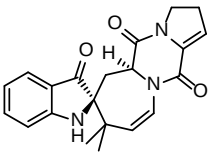
The structural complexity and skeletal diversity of natural products have served as inspirations to organic chemists for the discovery and design of new synthetic methods *en route* to their chemical synthesis. Our group focuses on the development of new methodologies that are specifically designed in the context a total synthesis of natural products of biological relevance. In this presentation, we wish to provide a comprehensive compilation of various novel transformations that have been developed in our group along with some salient aspects of the accomplished total synthesis.



Propolisbenzofuran B
(*2017*)

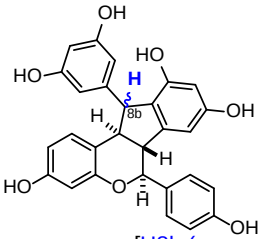


Integrastatine B
(*2016*)



Austamide

(*ongoing*)



Parvifolal A [H8b (β)]
Parvifolal B [H8b (α)]

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Invited Lecture (IL-47)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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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 NCL. At NCL, the focus of Ramana's group includes small molecules synthesis by employing transition metal complexes and developing new catalytic methods. 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 130 publications, 17 patents and 21 students have been awarded PhD. degree under his supervision.

HCN and H_2O: The Adam and Eve of Chemical Evolution?

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Abstract:
How life originated on earth is one of the most fundamental questions in science. There have been many hypotheses to explain its beginnings, but a general principle that everyone agrees upon is that the simpler the explanation, the more likely it is to be true. In my talk, I will discuss attempts in my group to approach this problem from an entirely fresh perspective – that of computational chemistry. Taking advantage of the recently developed *ab initio* nanoreactor (AINR) method, we have explored[1] an interesting question: what if the building blocks to RNA and proteins could have originated in early Earth from a single source of nitrogen and carbon: HCN, and a single source of oxygen: H_2O, under the same reaction conditions and in close proximity to one another? The results that we have obtained from this computational exploration are very interesting. We have found that, beginning from a mixture of HCN and H_2O molecules, we could obtain the precursors to RNA: cyanamide, glycolaldehyde and an oxazole derivative; as well as glycine, the precursor to proteins. Our work thus indicates that HCN and H_2O could have been the Adam and Eve of chemical evolution – the source of the precursor molecules that formed the basis of life on earth.

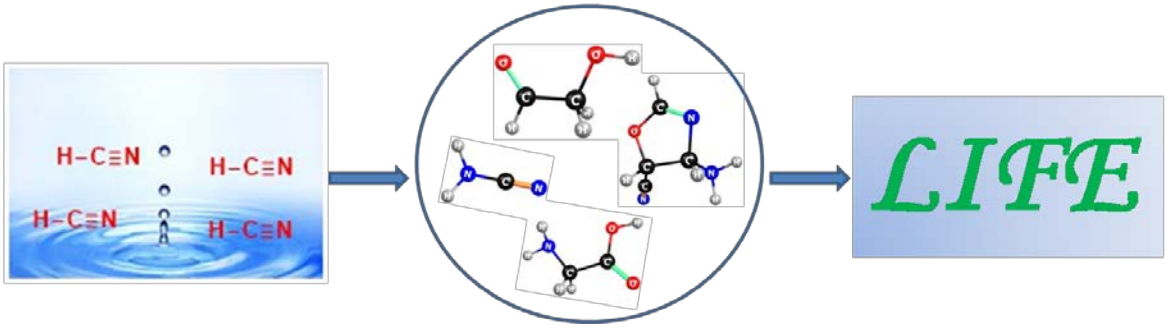

Figure 1. The interaction between HCN and H_2O: was it enough to give rise to life in early Earth?

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Invited Lecture (IL-48)

International Conference on Organometallics and Catalysis (ICOC 2020)

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Professional Experience

- 2008- Current- Scientist, National Chemical Laboratory, Pune, India
- 2005-2007 Post Doctoral Research Fellow (with Prof. Dr. Ward Thompson, Kansas University, Kansas, USA
- 2000-2004 Ph.D Student (with Prof. Dr. Tom Ziegler, University of Calgary, Alberta, Canada)
- 1997-2000 MSc. Student (with Prof. Dr. Tom Ziegler, University of Calgary, Alberta, Canada)
- Undergraduate studies from Indian Institute of Technology Kharagpur (IITK),West Bengal, India

Ligand-Enabled Au(I)/Au(III) Catalysis: New Opportunities in Cross-coupling Reactions

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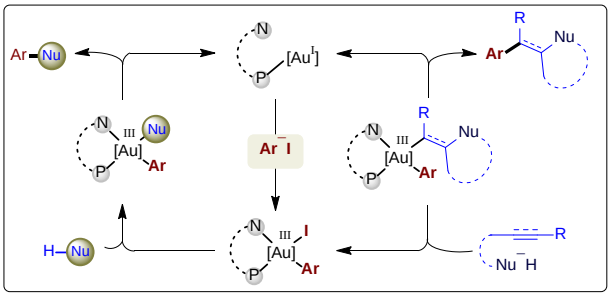
Abstract: The past two decades have remodeled the impression of gold from being an exorbitant glittery metal to the best catalyst for the activation and functionalization of various C–C multiple bonds. However, inspite of the reasonable efforts, the applicability of gold catalysis to the highly important cross-coupling reactions has remained highly limited. A prime reason for this is gold's reluctance to undergo the necessary oxidation state changes (Au: E^0 = +1.41 *vs* Pd: E^0 = +0.92 V) to catalyze cross-coupling reactions. With due credit to the pioneering work from the groups of Toste, Zhang, Hashmi and Glorius, two major strategies for achieving the inevitable Au(I)/Au(III) cycle have been developed which include: (a) External oxidant empowered Au(I)/Au(III) catalysis, (b) Au(I)/Au(III) Catalysis via merged gold/photoredox strategy.[1] Recently, our research group introduced an entirely new strategy wherein the use of benziodoxolones facilitates the Au(I)/Au(III) catalysis.[2]

In this presentation, I will be discussing a new mode of harnessing Au(I)/Au(III) catalysis wherein an ancillary P,N-ligand lowers the activation barrier for the oxidative addition of aryl halides to Au(I) and stabilizes the resulting Au(III)−aryl complex by P,N-coordination. The approach opens up new gateways for the development of enantioselective transformation by designing novel chiral P,N-ancillary ligands. Our explorations in the field of ligand-enabled Au(I)/Au(III) catalysis for achieving cross-coupling as well as 1,2-difunctionalization reactions of C-C multiple bond shall be discussed.[3]

Scheme 1. Gold-catalyzed reactions *via* ligand-enabled Au(I)/Au(III) catalysis



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Invited Lecture (IL-49)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Academic Qualification:

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- B.Sc. (**1992-1995**): North Maharashtra University, Jalgaon, India

Academic Qualification:

- Associate Professor (07/2017-till date): Department of Chemistry, IISER-Bhopal, Bhopal
- Senior Scientist (08/2013-06/2017): Division of Organic Chemistry, CSIR-NCL, Pune
- Senior Scientist (03/2011-08/2013): Organic Chemistry Division-II, CSIR-IICT, Hyderabad
- QRS (09/2008-03/2011): Organic Chemistry Division - II, CSIR-IICT, Hyderabad
- Research Fellow (01/2008-07/2008): The Scripps Research Institute, La Jolla, CA 92037, Advisor - **Professor K. C. Nicolaou**
- Research Fellow (06/2006-12/2007): Institute of Chemical and Engineering Sciences, Singapore, Advisor - **Professor K. C. Nicolaou**
- Assistant Professor (04/2005-03/2006): Department of Chemistry, Graduate School of Science, Tohoku University, Japan, Advisor - **Professor Yoshinori Yamamoto**
- JSPS Postdoctoral Fellow (11/2002-03/2005): Department of Chemistry, Graduate School of Science, Tohoku University, Japan, Advisor - **Professor Yoshinori Yamamoto**
- Postdoctoral Fellow (03/2002-11/2002): Institut für Organische Chemie, University of Goettingen, Germany, Advisor - **Professor Christoph Schneider**

His broad research interests include development of metal-, organo- and organo/metal-catalyzed enantioselective methods and total synthesis of natural products. He has been the recipient of SERB Distinguished Investigator Award – 2018, CRSI Bronze Medal-2018, INSA Young Scientist Medal – 2010, Alkyl Amines – ICT Foundation Day Young Scientist Award – 2010 and Avra Young Scientist Award - 2012. He was also elected as “Young Associate” of the Indian Academy of Sciences, Bangalore for the years 2010-2013.

Invited Lecture (IL-50)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

Dr. Biprajit Sarkar

Designation Professor and Chair

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Biprajit Sarkar grew up in Assam and studied chemistry at the University of Delhi and at the Indian Institute of Technology Bombay. At the end of 2001 he moved to the University of Stuttgart, Germany to work on his doctoral thesis with Prof. Wolfgang Kaim which he finished in 2005. After a one-year post-doctoral stay in the laboratory of Prof. Pierre Braunstein, Biprajit moved back to Stuttgart to work on his habilitation. On completion of his habilitation at the end of 2011, Biprajit was offered Professor's positions at the Technical University Dresden and at the Freie Universität Berlin. He decided to take up the latter offer and moved to the FU Berlin at the beginning of 2012. In 2018 he was offered a position at the University of Potsdam, which he declined and decided to stay on at the FU Berlin. The University of Stuttgart offered him a position as a chair of coordination chemistry in 2019. Biprajit decided to take up that offer and has been at the University of Stuttgart since October 2019. The research efforts of his group have been recognized by the selection of Biprajit as one of the "Rising Stars" at the ICCC 2014 in Singapore. He was awarded the Zasshikai Lectureship of the University of Tokyo in 2015. Since 2015 he has been a visiting professor at the IIT Bombay. His research interests are based on metal complexes of quinones, porphyrins/corroles, azo ligands, triazoles and mesoionic carbenes. Apart from synthetic chemistry, his group probes the utility of these metal complexes as magnetically and optically switchable molecular materials, as well as their utility in small molecule activation and catalysis.

Recent Advances in the Field of Pd-AAA Chemistry

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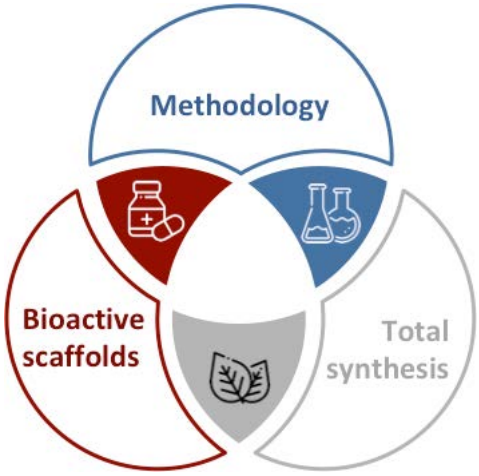
Abstract:
For the past several years, the group has focused on the development of new synthetic tools with a special emphasis given to structural and functional complexity. These methods span within the areas of organocatalysis, transition metal catalysis and, more recently, bio-hybrid catalysis. In this context, we've developed a number of palladium-catalyzed allylic alkylation processes and applied them to the synthesis of various chiral heterocyclic scaffolds.[1-6] I'll present here some of our recent results.



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Invited Lecture (IL-51)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Stellios Arseniyadis obtained his PhD from the University of Strasbourg (2002) under the supervision of late Dr Charles Mioskowski. He then joined Rhodia Chirex in Boston to work on various metal-catalyzed aryl bond-forming processes in collaboration with Professor Stephen L. Buchwald (MIT). After postdoctoral stays in the groups of Professors Alan C. Spivey (Imperial College London) and K. C. Nicolaou (The Scripps Research Institute), he became a permanent CNRS researcher at ESPCI Paris in 2005 where he was promoted to the rank of CNRS Director in 2015. The same year, he moved to Queen Mary University of London to start his own research group, which is principally involved in the development of new synthetic tools with a special emphasis given to asymmetric catalysis.

He is the recipient of the 2015 CNRS Bronze medal and the 2014 Thieme Chemistry Journal Award. He is a Fellow of the Royal Chemical Society and an elected member of the Organic Chemistry Division Bureau of the French Chemical Society.

Bio-Sketch of Speaker

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Studies & Positions

2017- Associate Professor (Docent), Eötvös Loránd University, Department of Organic Chemistry

2008-2017 Assistant Professor, Eötvös Loránd University, Department of Organic Chemistry

2007-2008 Faculty Member, Eötvös Loránd University, Department of Organic Chemistry

2005-2007 Postdoctoral Researcher, Eötvös Loránd University

2004-2005 Postdoctoral Fellow, Laboratory of Prof. Brian M. Stoltz, California Institute of Technology, Pasadena, California, USA.

2004 PhD., Eötvös Loránd University, Budapest, Hungary. Advisor: Dr. András Kotschy. Thesis: “Palladium catalyzed transformations in the synthesis of heterocycles”

2001-2003 PhD student at the Department of General and Inorganic Chemistry, Eötvös University, Budapest, Hungary

1999-2001 Industrial research. (Ubichem Ltd. Budapest, Hungary. GE Corporate Research and Development/Molecularis at Eötvös University)

1999 M. Sc. Chemist at Eötvös University, Budapest.

1988-1993 Secondary school, Irinyi János School, Budapest

Artificial Metalloenzymes: Challenges and Opportunities

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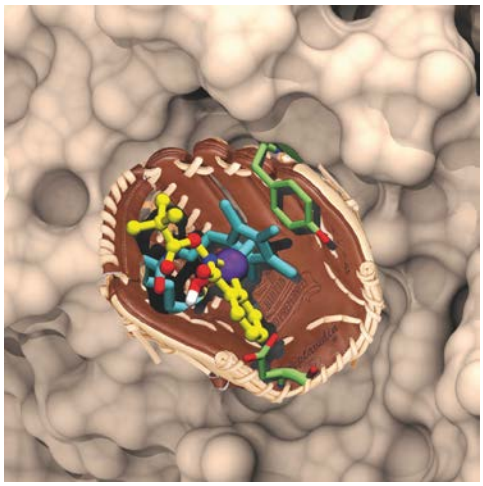
Abstract:
Artificial metalloenzymes result from the incorporation of a abiotic cofactor within a host protein. We and others have been exploiting the potential of the biotin-(strept)avidin technology for the creation of artificial metalloenzymes, Figure. Thanks to the remarkable supramolecular affinity of biotin for either avidin or streptavidin ($K_D > 10^{-13}$ M), linking of a biotin anchor to a catalyst precursor ensures that, upon stoichiometric addition of (strept)avidin, the metal moiety is quantitatively incorporated within the host protein. Alternatively, human carbonic anhydrase has proven equally versatile for the development of artificial metalloenzymes relying on aryl-sulfonamide anchors to ensure the localization of the abiotic metallocofactors within the host protein, Scheme.
The resulting artificial metalloenzymes can be optimized either by chemical (variation of the anchor-spacer-ligand moiety) or genetic- (mutation of the host protein) means. These chemo-genetic schemes were applied to optimize the performance for twelve different catalyzed transformations as well multiple reaction cascades in the presence of natural enzymes.[1]
More recently, we have been investigating the potential of artificial metalloenzymes for *in vivo* catalysis to complement metabolic pathways. In this context, *E coli*'s periplasm as well as surface display have proven particularly versatile to compartmentalize and evolve artificial metalloenzymes while maintaining the critical phenotype-genotype linkage



Scheme: Artificial metalloenzymes result from the anchoring of an organometallic cofactor within a protein scaffold.

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Invited Lecture (IL-53)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Thomas R. Ward was born in Fribourg in 1964 as the last of 6 children of John E. Ward and Ada Lovinger Ward. He received his diploma in Chemistry in 1987 from the University of Fribourg with organic chemistry as major and inorganic chemistry as minor subjects.
From 1988 to 1991, he was a doctoral student in the group of Prof. L. M. Venanzi at the ETH Zürich in close collaboration with Prof. D. Seebach. His PhD thesis dealt with the synthesis and coordination properties of C3-symmetric phosphine ligands and their use as acetalization catalysts. This work benefited from a fruitful collaboration with Ciba Geigy which patented these systems.
Fascinated by group theory, he joined the group of Prof. R. Hoffmann at Cornell University as a Swiss National Science postdoctoral fellow (1991-1992). This theoretical excursion led him into the fascinating field of heterogeneous catalysis: Why is rhodium so efficient at removing NO from car exhaust?
Soon after returning to Switzerland for a second postdoc in the group of Prof. C. Floriani at the University of Lausanne, he was awarded the A. Werner Fellowship and moved to Berne to undertake his independent career in Fall 1993. He obtained his Venia Legendi in 1999 and moved to the University of Neuchâtel in Fall 2000. After seven years spent at the University of Neuchâtel, he moved to the University of Basel in March 2008. The group research is centered on the exploitation of proteins as host for organometallic moieties with applications in catalysis as well as in nanobiotechnology.
He is happily married to Anouck and are both very proud of their three children: Benjamin Roald (1994), Samuel (1996) and Elise (1999).
Thomas R. Ward was awarded the ETH Medaille (1991), the A. Werner Fellowship (1993) as well as the A. Werner Prize (1998) and a Swiss National Science Foundation Förderungsprofessur (2000). In 2005, he was awarded the medal of the Czech Academy of Sciences for his research on artificial metalloenzymes based on the biotin-avidin technology. In 2016, he was awarded an advanced ERC grant to realize his DrEAM: the *Di*rected *E*volution of *A*rtificial *M*etalloenzymes.
He is the director of the NCCR Molecular Systems Engineering

Invited Lecture (IL-54)
International Conference on Organometallics and Catalysis (ICOC 2020)

Rhodium-Catalyzed Addition of Pronucleophiles to Alkynes and Allenes: An Atom-Efficient Alternative to the Tsuji-Trost Reaction

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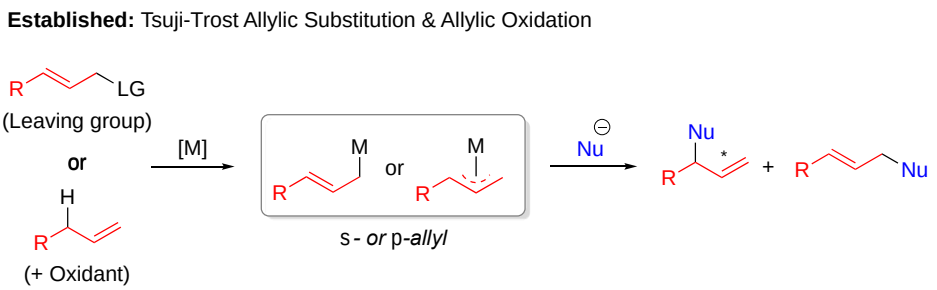
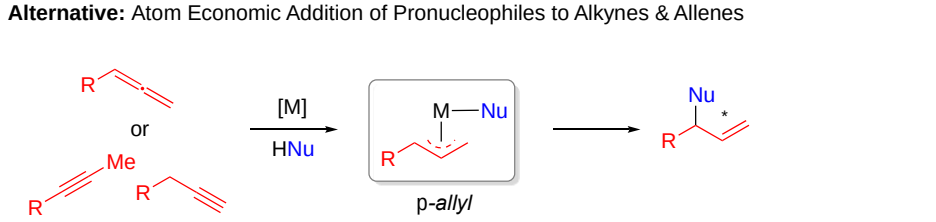
Abstract:
Transformation of simple and readily accessible starting materials to branched allylic derivatives is an important topic in organic synthesis because of the versatility of the allylic moiety for further elaboration and the stereogenic center for asymmetric synthesis.[1] In the last decades, significant progress toward this goal has been achieved, in particular with allylic substitution[1] and allylic C-H oxidation[2] chemistry. However, these methods require pre-installation of a leaving group or stoichiometric amounts of an oxidant, respectively.





As an alternative to these methods, we have developed a set of new reactions enabling the addition of pronucleophiles to alkynes and allenes furnishing branched allylic derivatives in a completely atom-economic fashion under neutral conditions. By choice of the right catalyst, a wide range of regio- and stereoselective C/O, C/N, C/S and C/C-bond-forming reactions could be achieved.[3,4] Applications in target-oriented synthesis will also be presented.

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Invited Lecture (IL-54)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Bernhard Breit is a graduate of the University of Kaiserslautern (Diploma, Dr. rer. nat.). After postdoctoral studies at Stanford University he joined the faculty at the University of Marburg for his habilitation and was appointed Professor of Organic Chemistry at the University of Heidelberg. He is presently a Professor of Organic Chemistry at the Albert-Ludwigs-Universität in Freiburg. Professor Breit's research in organic synthesis and catalysis encompasses pioneering studies on supramolecular concepts in homogeneous catalysis and the development of new catalytic atom-economic bond forming reactions. He is author of more than 250 publications.

Invited Lecture (IL-55)
International Conference on Organometallics and Catalysis (ICOC 2020)

Carboxylates as Deciduous Directing Groups in C–H Functionalizations

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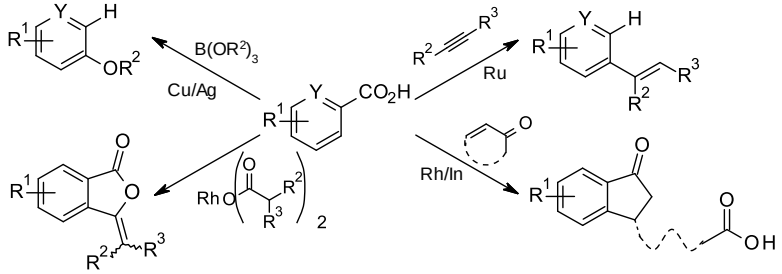
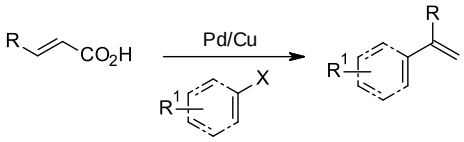
Abstract:

Over the past decade, carboxylic acids have become established as versatile substrates for catalytic transformations. Various activation modes have been achieved, such as catalytic additions across multiple bonds, decarbonylative and decarboxylative couplings, C–OCOR activations and C–H functionalizations. This presentation focuses on the use of carboxylates as deciduous directing groups, which stay in place just long enough to direct a C–H functionalization reaction into a specific position and are shed tracelessly as soon as the new C–C or C–heteroatom bond has formed.



Scheme 1: C–H functionalization reactions starting from aromatic carboxylates.

In the carboxylate-directed, Ag/Cu-catalyzed C–H alkoxylation,[1] an alkoxide group is introduced in the ortho position of aromatic carboxylates. The new substituent destabilizes the C–COOH bond to an extent that protodecarboxylation occurs, precluding further substitution of the second ortho-C–H bond. This way, benzoic acids are selectively converted into aryl alkyl ethers. In the Ru-catalyzed decarboxylative hydroarylation of alkynes with benzoic acids, the carboxylate group directs the C–H functionalization step into its ortho-position and is liberated as CO_2 in a concerted C–C bond-forming step.[2] In the presence of a Rh/In catalyst, benzoic acids react with α,β-unsaturated ketones with formation of two new C–C bonds along with the selective cleavage of non-activated C–H, CO–OH, and C–COR bonds. The resulting annelation opens up a versatile synthetic entry to functionalized indanones.[3]



Scheme 2: Synthesis of vinyl arenes from α,β-unsaturated carboxylic acids.

Carboxylates also act as deciduous direction groups in the regiospecific synthesis of 1,1-disubstituted alkenes from α,β-unsaturated carboxylic acids and aryl halides, as well as in the selective synthesis of vinyl arenes from acrylic acids.[4]

References and Notes:

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3. G. Zhang, Z. Hu, F. Belitz, Y. Ou, N. Pirkl, L. J. Gooßen, *Angew. Chem. Int. Ed*. **2019**, *131*, 6501-6505.
4. a) J. Tang, D. Hackenberger, L. J. Gooßen, *Angew. Chem. Int. Ed.* **2016**, *55*, 11296–11299; b) Y. Gao, Y. Ou, L. J. Gooßen, *Chem. Eur. J.* **2019**, *25*, 8709-8712.

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Lukas Gooßen studied Chemistry at the universities of Bielefeld and Michigan and conducted his Master's research in the group of K.P.C. Vollhardt at UC Berkeley. He was awarded a Ph.D. in 1997 for research on *N*-heterocyclic carbene complexes supervised by W.A. Herrmann at TU Munich, and pursued postdoctoral research with Nobel laureate K.B. Sharpless. He began his professional career as an industrial chemist at Bayer AG in 1999, then moved back to academia to the group of M.T. Reetz, MPI for Coal Research for his Habilitation, and further to RWTH Aachen. From 2005-2016, he was professor at TU Kaiserslautern. In 2016, Lukas Gooßen was appointed Chair of Organic Chemistry at RU Bochum.
His research is devoted to the development of novel concepts for C–C- and C–heteroatom bond formation designed to reduce the production of waste salts and effluents. He received the Jochen-Block award of the DECHEMA (2003), the Carl-Duisberg Award of the GDCh (2007), the Novartis Young Investigator Award (2007), and the AstraZeneca Award in Organic Chemistry (2008).

Organometallics Meet Emergence: A Molecular Approach to the Evolution of Electrocatalysts

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Abstract

The low-temperature synthesis of inorganic materials and their interfaces at the atomic and molecular level provides numerous opportunities for the design and improvement of inorganic materials in heterogeneous catalysis for sustainable chemical energy conversion or other energy-saving areas. The transformation of molecules to materials is an emergence phenomenon, that is, the process creates novel complex properties of the resulting material entities which are absent in the starting material. Using suitable organometallic single-source precursors for functional inorganic nanomaterial synthesis allows for reliable control over uniform particle size distribution, stoichiometry which can help to reach desired chemical and physical properties.[1] In my talk, I would like to outline main achievements and challenges of the molecular precursor approach in light of selected recent developments of molecule-to-nanomaterials synthesis for renewable energy applications, relevant for the oxygen evolution reaction (OER), hydrogen evolution reaction (HER) and overall water-splitting. Electrochemical water-splitting into hydrogen (H_2) and oxygen (O_2) is widely regarded as a promising approach to producing environmentally-friendly fuel for future energy supply. In the recent years, inexpensive, earth-abundant and environmentally benign transition-metal oxides, hydroxides and other functional materials in conjunction with semiconducting co-catalyst that can independently catalyze OER and HER have been established.[2] Still the major challenge is to provide reliable catalyst systems for HER, OER and overall water-splitting which are highly efficient, robust and long-term stable (at least for several month without loosing activity). The advantage of using the molecular precursor approach to provide innovative solutions will be discussed.

Acknowledgment:
We thank the Deutsche Forschungsgemeinschaft (Cluster of Excellence UniSysCat), BMBF (project MANGAN), and the Einstein Foundation Berlin for financial support.

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2. P. W. Menezes, A. Indra, I. Zaharieva, C. Walter, S.n Loos, S. Hoffmann, R. Schlögl, H. Dau, M. Driess, *Energy Environ. Sci.* **2019**, 12, 988-999.

Invited Lecture (IL-56)

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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His research foci are (http://www.driess.tu-berlin.de/)

- New functional groups in main-group chemistry, activation of unreactive bonds in small molecules with them, in particular based on silicon compounds (divalent species, stable silanones, silicon(0) complexes)
- Electron-rich silicon-based steering ligands for transition-metal mediated homogeneous catalysis
- Activation of small molecules (e.g., dihydrogen, dioxygen, ammonia and alkanes) through bioinspired transition-metal complexes, including model complexes of copper-, nickel- and iron-based oxygenases.
- Metalorganic single-source precursors for the low-temperature synthesis of nanoscaled functional materials for energy-saving key technologies like catalysis (materials for solar and electrocatalytic water splitting) and for optoelectronics, including präorganized synthesis of multinary basis materials Basismaterialien for energy-saving thin-film field effect transistors
- Molecular models for heterogeneous (e.g., metal oxide-based selective oxygenation of hydrocarbons) and bioinorganic catalysts (e.g., hydrogenases, oxygenases, superoxidases)

Invited Lecture (IL-57)
International Conference on Organometallics and Catalysis (ICOC 2020)

Hybrid Catalysis for Dehydrogenation and Asymmetric C–C Bond-Formation

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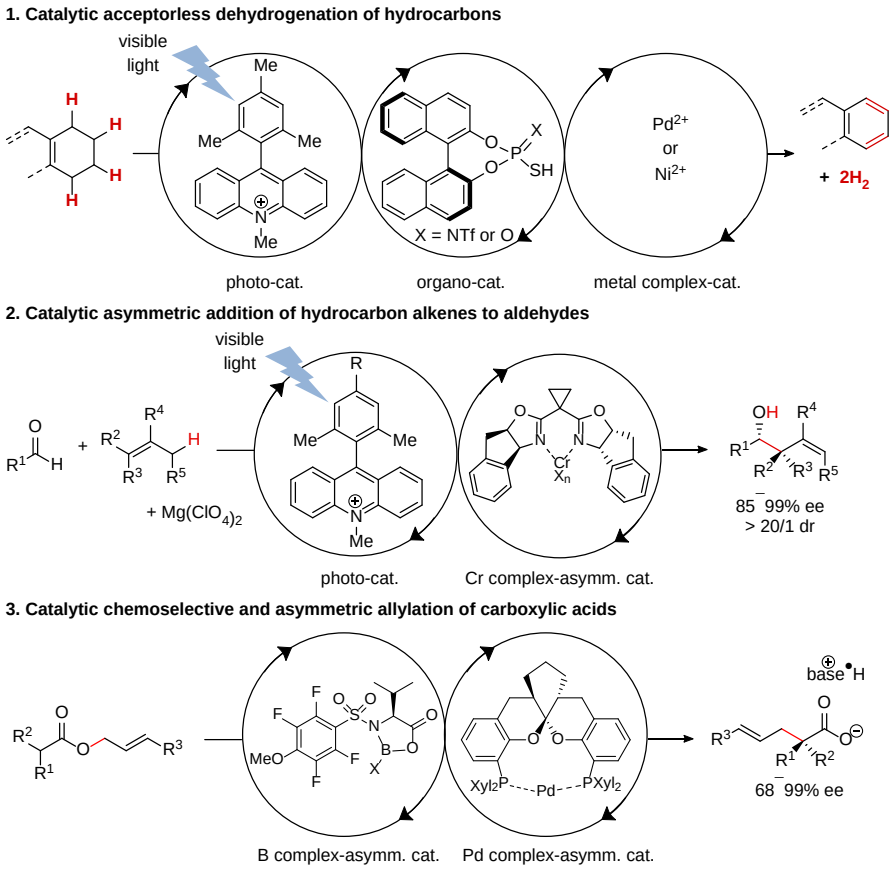
Abstract:
Hybrid catalysis, a multicatalytic system involving catalysts with distinct individual functions, is an emerging concept. Integrating the functions of multiple catalysts, hybrid catalysis will enable molecular synthesis of high efficiency, starting from abundant organic molecules such as hydrocarbons. I will discuss three topics here: 1. a ternary hybrid catalysis comprising a photo-catalyst, an organocatalyst, and a metal complex catalyst (Pd or Ni) promoting acceptorless dehydrogenation of hydrocarbons (eq. 1) [1]; 2. a binary hybrid catalysis comprising a photo-catalyst and a chiral chromium complex catalyst promoting an asymmetric addition of alkenes to aldehydes (eq. 2) [2]; and 3. a binary hybrid catalysis comprising chiral boron and palladium catalysts promoting a chemoselective and asymmetric α-allylation of carboxylic acids (eq. 3) [3].



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Invited Lecture (IL-57)

International Conference on Organometallics and Catalysis (ICOC 2020)

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Motomu Kanai was born in 1967 in Tokyo, Japan, and received his bachelor degree from The University of Tokyo (UTokyo) in 1989 under the direction of late Professor Kenji Koga. He obtained an assistant professor position in Osaka University under the direction of Professor Kiyoshi Tomioka in 1992. He obtained his PhD from Osaka University in 1995. Then, he moved to University of Wisconsin, USA, for postdoctoral studies with Professor Laura L. Kiessling. In 1997, he returned to Japan and joined Professor Masakatsu Shibasaki's group in UTokyo as an assistant professor. After doing lecturer (2000–2003) and associate professor (2003–2010), he is a professor in UTokyo (since 2010). He acted as PI of ERATO Kanai Life Science Project (2011–2017), and is acting as the head investigator of MEXT Grant-in-Aid for Scientific Research on Innovative Areas, "Hybrid Catalysis" (2017–2022). He has received The Pharmaceutical Society of Japan Award for Young Scientists (2001), Thieme Journals Award (2003), Merck-Banyu Lectureship Award (MBLA: 2005), Asian Core Program Lectureship Award (2008 and 2010, from Thailand, Malaysia, and China), Novartis Lecturer in Organic Chemistry (2011), Thomson-Reuters the 4th Research Front Award (2016), and Nagoya Silver Medal (2020). His research interests entail design and synthesis of functional molecules.

FLASH TALK

Ultrathin Nanosheets: 3D to 2D Journey of Water Splitting Catalysts

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Abstract:

Designing efficient catalyst system for the anodic water oxidation requires the knowledge of the active catalytic sites during the electrochemical process. X-ray absorption (XAS) studies revealed that cobalt based catalysts are transformed into $Co(O)_x(OH)_y$ active structure during alkaline water oxidation in anode.[1-4] Therefore, designing of the $Co(O)_x(OH)_y$ is important to attain improved electrochemical water oxidation activity. Here, the synthesis of ultrathin $Co(O)_x(OH)_y$ nanosheets from different metal organic frameworks (Prussian blue analogue, zeolitic imidazolate framework) has been described by electrochemical anodic oxidation (**Figure 1**). Ultrathin $Co(O)_x(OH)_y$ nanosheets showed excellent water oxidation activity (< 250 mV overpotential to reach 10 mA cm^{-2} current density) and excellent stability for 100 h of continuous oxygen production. Operando XAS studies revealed that potential dependent deprotonation of $Co(O)_x(OH)_y$ led to attain high oxidation state (+3.2) of Co during water oxidation.

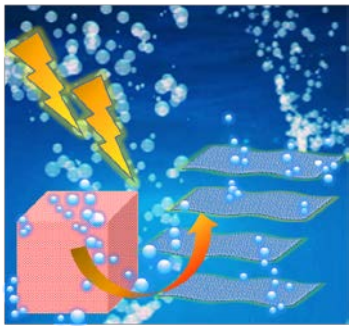

Figure 1. Schematic representation for the transformation of metal organic frameworks to ultrathin cobalt(oxy)hydroxide nanosheets with applied anodic potential.

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Keywords:

2D materials; ultrathin nanosheets; cobalt (oxy)hydroxide; water splitting, reaction mechanism

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Arindam Indra is an assistant professor in the department of Chemistry, IIT (BHU), Varanasi (India). He received his Ph.D. degree from IIT Bombay (India) in mesoporous silica supported organometallic catalysis. He joined Technische Universität Berlin (Germany) as a postdoctoral fellow and developed the basic concept of structure-activity relationship in water oxidation catalysts. As an assistant research professor in Hanyang University (Republic of Korea), he worked in the field of self-supported catalyst systems for electrochemical water splitting. Currently, his group designs metal organic framework (MOF) derived functional materials for energy conversion and organic reactions.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

α-Nitro-*α,β*-Unsaturated Ketones: An Electrophilic Acyl Transfer Reagent in Catalytic Asymmetric Friedel-Crafts and Michael Reactions

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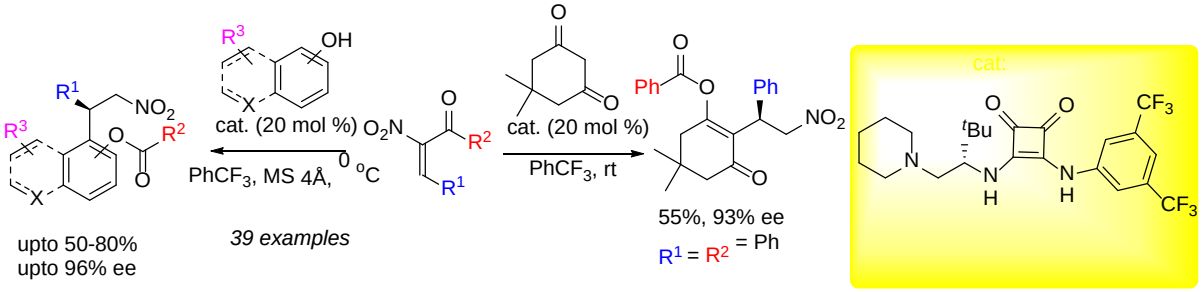
Abstract:
We introduce *α*-nitro-*α,β*-unsaturated ketones as efficient electrophilic acyl transfer reagent and were employed in Friedel-Crafts as well as in Michael reactions. The desired acyl transfer products of these reactions were obtained in high yields with high to excellent enantioselectivities with *t*-leucine derived squaramide catalyst under mild reaction conditions. Few applications including a synthesis of isoxazoline motif have been demonstrated.

Scheme:



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Professor Subhas Chandra Pan obtained his B.Sc. degree in Chemistry Honours in 2001 from Calcutta University and M.S. degree in 2004 from Indian Institute of Science, Bangalore. During his MS thesis he worked in Prof. Goverdhan Mehta's laboratory on the total synthesis of epoxyquinone natural products. He obtained his PhD degree in 2008 under the guidance of Prof. Benjamin List at the Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany. After doing postdoctoral studies at Harvard University with Prof. E J Corey and at the Scripps Research Institute, Florida with Prof. Glenn C. Micalizio, he joined IIT Guwahati as Assistant Professor in 2011 and was promoted to Associate Professor in 2015 and to Full Professor in 2019.
He recieved DAE Young Scientist Research Award 2012 and Thieme Chemistry Journal Award 2018.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

The curious case of a labile C-C bond

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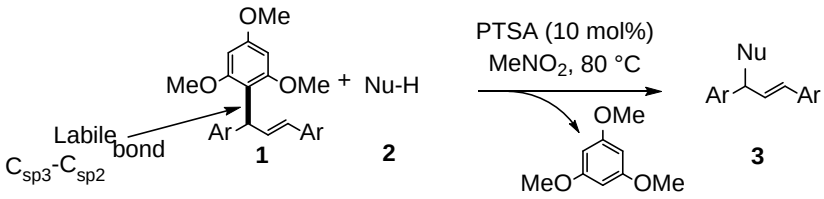
Abstract:
The thermodynamic stability of the C-C bond has not only made it ubiquitous but also has narrowed the avenue in literature that explores the cleavage of C-C bonds. Conventionally, the sparse collection of C-C bond breaking reactions exploits one or more of these three susceptibilities, i) release of ring strain; ii) chelation assistance; iii) cleavage of stable functional fragments such as allyl, carbonyl, cyano etc.[1-3] Recently a lot of interests have been focussed on the cleavage of stable carbon-based fragments in a bid to develop efficient leaving groups for application in organic syntheses. In this regard we have previously reported the potential of 2,4,6-trimethoxyphenyl moiety as a carbon-based leaving group in organic syntheses.[4,5]

Herein, we have found that a 2,4,6-trimethoxyphenyl group can easily be exchanged from allylic systems by various nucleophiles through the cleavage of the C_{sp3}-C_{sp2} bond (Scheme 1). Nucleophiles such as indoles, 4-hydroxycoumarin, 4-methoxythiophenol etc. reacts smoothly to generate the corresponding derivatives in good yields while generating 1,3,5-trimethoxybenzene as the by-product. The substitution reaction takes place in mild reaction conditions in presence of an acid. We have also noted that in absence of a nucleophile, intramolecular substitution takes over to replace the significantly labile C_{sp3}-C_{sp2} bond. We have carried out several control reactions and spectroscopic monitoring to gauge the mechanism underlying the bond breaking reaction.



Scheme 1: Robust C_{sp3}-C_{sp2} bond turns labile in acidic medium.

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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Paresh Nath Chatterjee completed his B.Sc. from Ramakrishna Mission Vidyamandira (under Calcutta University) and M.Sc. from Calcutta University, West Bengal. After completing masters, he joined the research group of Prof. Sujit Roy at Indian Institute of Technology Kharagpur and completed his Ph.D. in the area of "Organometallics and Catalysis" under the joint supervision of Prof. Sujit Roy and Prof. Manish Bhattacherjee. After Ph. D., Dr. Chatterjee joined National Institute of Technology Meghalaya as Assistant Professor in 2013 as the first faculty of the department. His current research interest includes both homogeneous and heretogeneous catalysis in the domain of C-C bond making and breaking reactions.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Stereoselective Desymmetrization of *meso*-Cyclohexadienones to Access Complex Molecules

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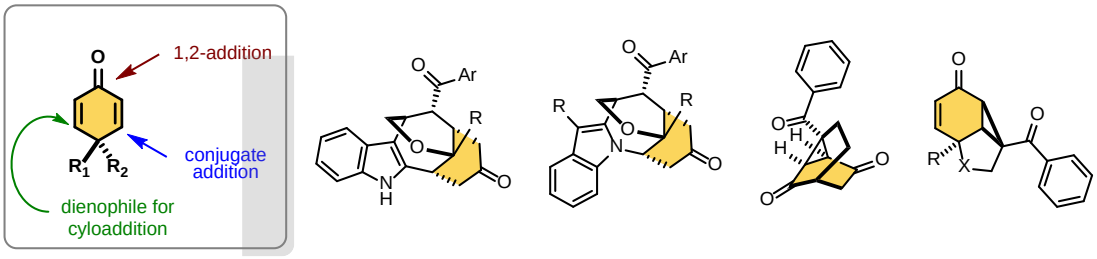
Abstract:
Desymmetrization of symmetric molecules is one of the most powerful tool en route to efficient diastereo- and enantioselective syntheses of biologically active complex molecules. Several potential advantages associated with the desymmetrization of prochiral compounds and these starting substrates are often easy to prepare. In continuation of our effort on the desymmetrization, we have developed various stereoselective approaches on cyclohexa-2,5-dienones for the construction highly factionalized scaffolds in our laboratory and details will be presented.



Scheme: Desymmetrization *meso*-cyclohexa-2,5-dienones

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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Transition Metal-Catalyzed C–H Functionalization/Annulation Cascade for the Synthesis of Spiroheterocycles

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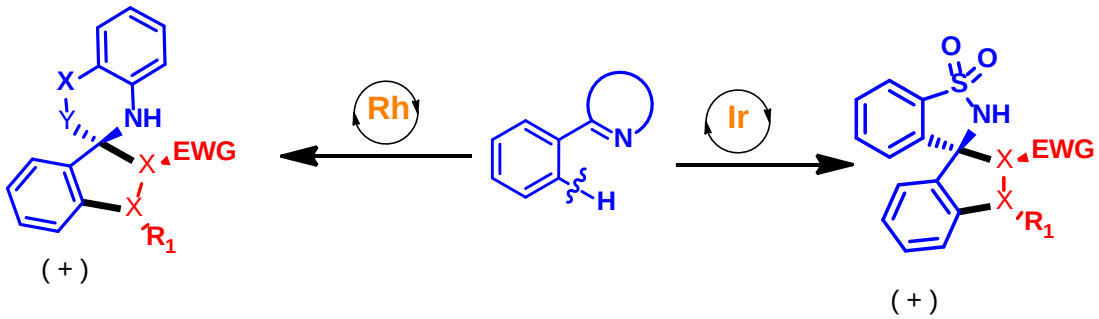
Abstract:
Benzosultam, benzoxazine and quinazolinone are considered as privileged pharmacophores in medicinal chemistry and therefore functionalization of these scaffolds is considered as of exorbitant importance. Recently, we have developed Rh and Ir catalyzed mild and efficient redox-neutral methodologies*via* direct and selective activation of relatively inert C□H bonds followed by coupling with nitroalkenes /activated olefins in regio and stereoselective manner for the synthesis of densely functionalized potential bioactive spiroheterocycles.



Scheme 1: Abstract of the work

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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Dr. Indubhusan Deb obtained his M.Sc. degree in organic chemistry from Banaras Hindu University. He completed his Ph.D in 2008 at the Indian Institute of Technology Bombay (IITB) under the supervision of Professor I. N. N. Namboothiri. Thereafter, he moved to Rutgers University, USA to carryout postdoctoral research with Professor Daniel Seidel where he was involved in doing research for the synthesis of chiral heterocycles. After spending three years at Rutgers, he joined in the group of Professor Naohiko Yoshikai at Nanyang Technological University, Singapore, for his 2nd postdoctoral research. In April, 2013 He joined as a research investigator (Project leader) in process chemistry division of Bristol Myers Squibb Research canter in Bangalore. Dr. Deb joined as a senior scientist in the division of Organic and Medicinal Chemistry at CSIR-IICB, in Jan, 2014. His research group is actively involved in asymmetric synthesis and designing synthetic methodology employing transition metal–catalyzed C-H bond activation chemistry for the synthesis of potential bioactive small molecules.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Regioselective C(sp^3)-Methylation, Alkylation and Arylation *via* C(sp^3)-H Activation

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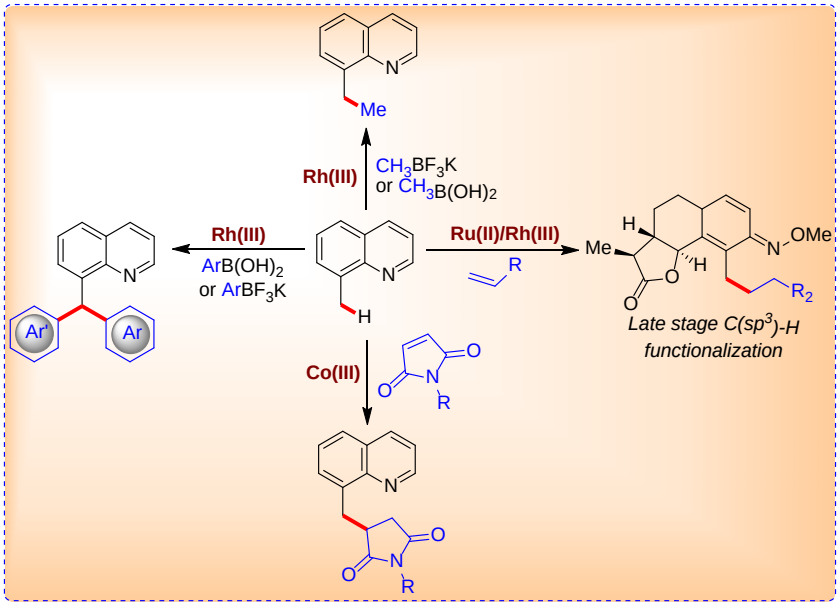
Abstract:
Nitrogen-containing heterocycles are of utmost importance due to their broad range of biological activities. Among them, quinolines are mainly known for their antimalarial potential and due to parasite resistance to many of the current antimalarial drugs, efforts are being made worldwide to synthesize new quinoline derivatives with better activity.[1] In last five years our group have synthesized various new quinolines derivatives [C8-derivatives *via* metal-catalyzed C-H activation, and C-2 / C-3 derivatives under metal-free conditions].[2,3] Recently, we turned our attention towards functionalization of quinolines *via* C(Sp^3)-H activation where regioselective methods were developed for C(sp3)-methylation, alkylation and arylation.[4] Our aim is to contribute further by succeeding in the functionalization of quinolines under mild reaction conditions through proper understanding of the reaction pathway.



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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Dr. Sharma natively from Himachal Pradesh completed his Ph.D. from CSIR-IHBT, Palampur / GNDU, Amritsar. After that, he did two postdocs, first with Prof. D. Maiti, IIT, Bombay and second with Prof. Sukbok Chang, KAIST, South Korea. Dr. Upendra Sharma started his independent research in the fall of 2014, and his group research focus involves transition-metal-catalyzed remote C-H activation/functionalization and natural product chemistry. Mainly his group is looking for new antimalarial molecules either through metal-catalyzed modification of quinolines or from natural sources. In 2016, Dr. Sharma got the Thieme Chemistry Journal Award and Manjushree Pal Memorial Award for Best Oral Presentation from Ethanopharmacology Society of India, Kolkata in 2017. Currently, he is an Early Career Advisory Board member in the *Asian Journal of Organic Chemistry*. He has published >100 research articles in reputed international journals and filed three patents till date.

High-Valent Metalloporphyrinoid Stability and Reactivity

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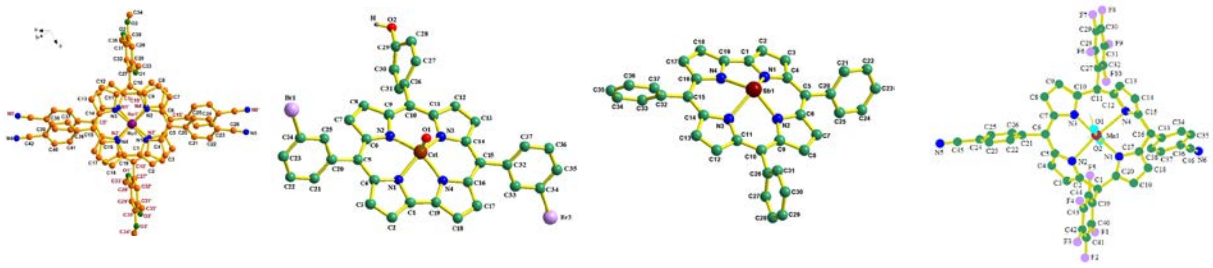
Abstract:
Porphyrinoids are the most prominent ligands used in metal complex mediated organic transformation reactions. The most common example is the Cytochrome P450 with iron porphyrin as its cofactor. In many cases where the use of other ligands is not feasible, porphyrinoids remain as the only viable choice. Over past few decades, tetrapyrrolic macrocycles other than porphyrin, like core-modified porphyrinoid are considerably optimized and developed. Corrole ring is just one *meso*-carbon shorter than related porphyrin macrocycle. Compared to porphyrin which has two imino hydrogens, corrole contains three imino hydrogens. Therefore it can act as a trianionic ligand. Due to the smaller cavity size and more anionic nature of corrole, it tends to stabilize metals in higher oxidation states. In majority of the cases, in the native state, the oxidation state of metal is one unit higher in metallo-corrole than its metallo-porphyrin analogue. Thus it has been proven to be easier and more realistic to study the higher oxidation states of metal in corrole based macrocycle. Attempts have been made to explore various scaffolds of corrole frameworks and their corresponding metal derivatives on the basis of either biological or physical significances. Efforts are laid to comprehend the mechanistic aspects of their reactivity and also electronic, structural, morphological and spectroscopic changes in individual cases. In this lecture, recent results from my group will be presented [1-5].



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Flash Talk & Poster Presentation

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Dr. Sanjib Kar moved to the Burdwan University for his Bachelor studies and to Kalyani University for his Master's. At the middle of 2001, Dr. Kar moved to IIT Bombay where he worked on his PhD with Prof. G. K. Lahiri. Having successfully finished his PhD in December 2005, Dr. Kar moved to Institute for Materials Chemistry and Engineering (*IMCE*), Kyushu University in Japan as a JSPS post-doctoral fellow with Professor Yoshinori Naruta. At the beginning of 2009, Dr. Kar joined NISER-Bhubaneswar as an assistant professor and presently he is an Associate Professor in NISER-Bhubaneswar. His group's major research interests include: i) Syntheses and functionalization of corrole macrocycles, ii) corrole metal complexes for metallo-enzyme mimicry, and iii) the design, synthesis and applications of metallo-corrole based supramolecular *nano*-architectures.

Nitrosoarene Chemistry: From Reagent to a Catalyst

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Abstract:
It's really astounding that the nitrosoarene chemistry still can deliver so much exciting transformations. Nitrosoarenes are mainly applied in Nitroso Diels Alder reactions (NDA) as a synthon for amino-alcohols after cleaving the N–O bond. Organocatalysis utilizes nitroso-aldol reactions for regioselective α-amination or α-hydroxylation of carbonyls. We will discuss our discovery on nitrosoarene chemistry either via polar or via a radical pathway. A diverse set of new functionalities produce in a metal-free condition symbolizing the advantage of this strategy headed for the synthesis of medicinally important analogous.[1]

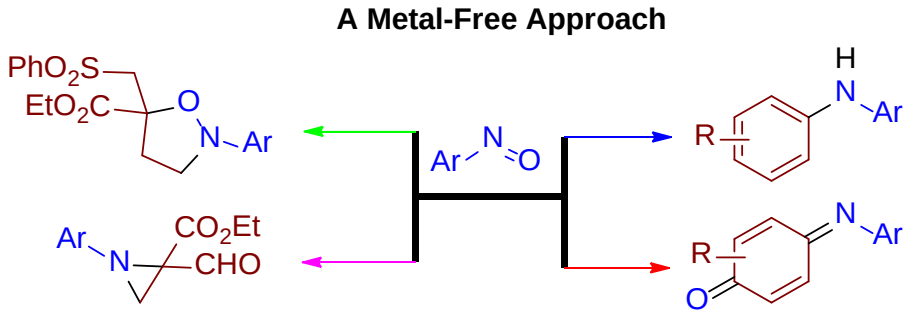

Figure 1: Application of Nitrosoarenes for the diverse synthesis in a metal-free pathway.

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Bio-Sketch of Speaker

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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.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Unified Strategies for Nickel-Catalyzed C–H Functionalization of Indoles: Scope and Mechanistic Aspects

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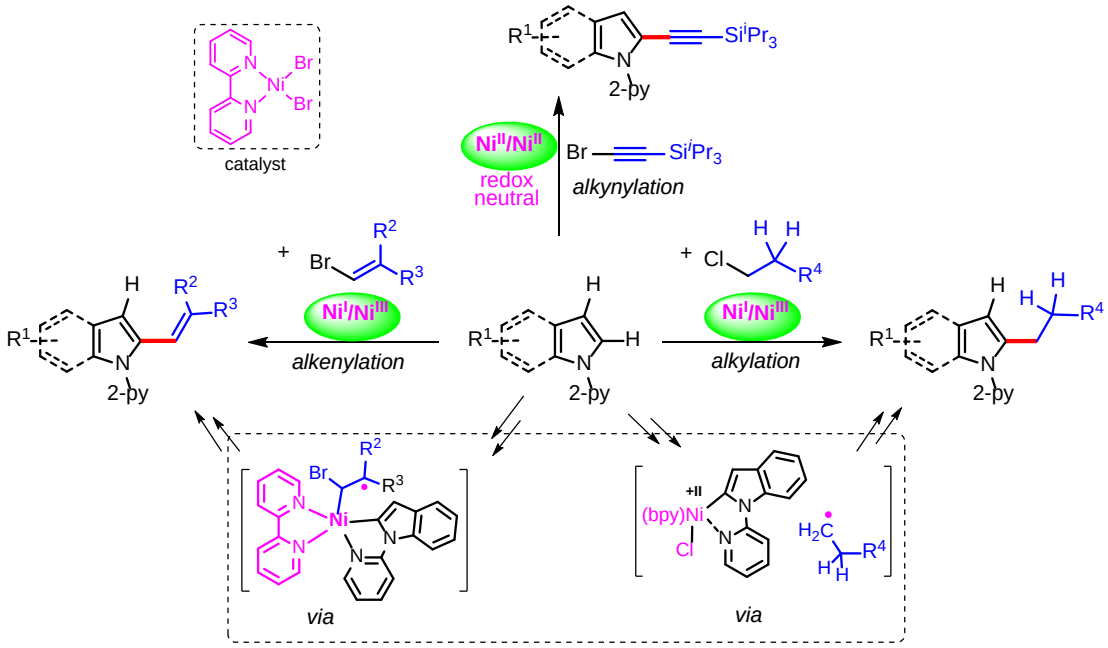
Abstract:
Selective C−H bond functionalization of heteroarenes, particularly indoles, by the catalyst based on earth-abundant metals, such as nickel has drawn considerable attention. To this end, our research activities have been focused on the design and development of suitably ligated nickel catalysts for selective functionalization of indoles with the assistance of a monodentate-chelate auxiliary (Scheme 1).[1-6] In this presentation, Ni-catalyzed regioselective C–H alkylation, alkenylation and alkynylation of indoles will be discussed. Applicability of the methods for the synthesis of biologically active coumponds will be highlighted. In addition, the focus will be paid towards the mechanism of these reactions. As will be shown, the alkylation and alkenylation follow a Ni(I)/Ni(III) pathway, whereas alkynylation proceeds *via* a redox neutral process. Overall, a comprehensive catalytic scope and mechanism of the Ni-catalyzed functionalization of indoles will be discussed.



Scheme 1: Nickel-Catalyzed Indole Functionalization.

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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Education: M. Sc. Sambalpur University, Odisha (Organic Chemistry Specialization)
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2007-2010 NSF-CENTC Post-doctoral study with Prof. Alan S. Goldman, Rutgers University, New Jersey, USA

2010-2011 Alexander von Humboldt Post-doctoral fellows with Prof. Lutz Ackermann, University of Göttingen, Germany

2011-2015: Senior Scientist, NCL, Pune

2015-till date: Principal Scientist, CSIR-NCL, Pune

Awards: R.C. Tripathy Young Scientist Award, OCS, Odisha
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Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Photoredox Catalyzed Cascade Radical Annulations Involving *N*-(acyloxy)phthalimides: Towards Alkylated Heterocycles

Sanju Das, Sushanta Kumar Parida, Tanumoy Mandal, Laxmikanta Sing, Suman De Sarkar* and Sandip Murarka*

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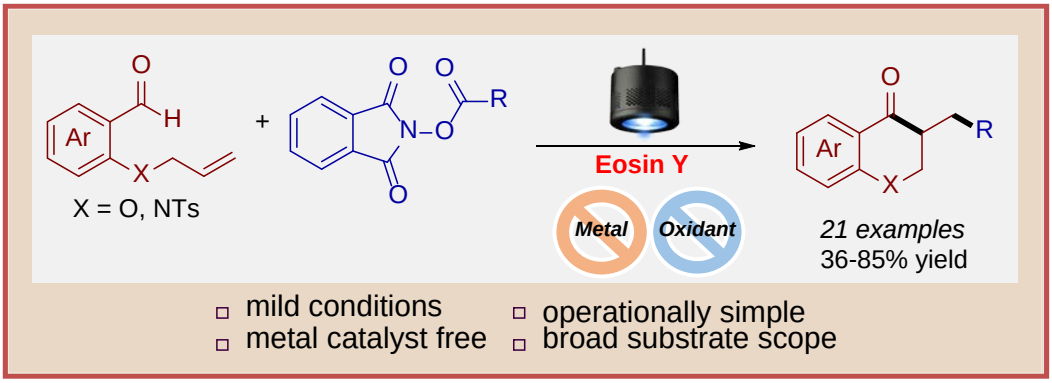
Abstract:
The chroman-4-one framework belongs to the privileged class of heterocycles and constitutes an integral part of numerous natural products, pharmaceuticals and biologically active compounds. Considering significant applications of chroman-4-ones, it is needless to mention that the development of straightforward, milder and environmentally benign approaches for the synthesis of this scaffold is highly desired. Accordingly, a Eosin Y catalyzed efficient and robust approach for the synthesis of 3-alkyl substituted chroman-4-one scaffold is developed using visible light induced radical cascade cyclization strategy. Importantly, the presented metal-free technology also allowed an efficient access to alkylated 2,3-dihydroquinolin-4-ones in good yields. The reaction is initiated through the generation of alkyl radicals from *N*-(acyloxy)phthalimides under photoredox conditions, which subsequently undergo intermolecular cascade radical cyclization on 2-(allyloxy)arylaldehydes to afford chroman-4-one scaffolds. The presented strategy is attractive with regard to mild reaction conditions, operational simplicity, high functional group tolerance and broad substrate scope.



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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Sandip Murarka pursued his PhD from WWU Münster, Germany under the supervision of Prof. Armido Studer. In 2013, he moved to Max Planck Institute of Molecular Physiology, Dortmund to work as a postdoctoral research fellow in the laboratory of Prof. Herbert Waldmann. Since, May 2017 he is holding the position of an Assistant Professor at the Indian Institute of Technology Jodhpur, India. His current research activities include study of novel activation modes and development of chemoselective and sustainable transformations towards the synthesis of interesting molecular architectures.

TALENTED TIN(II)

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Abstract:
We will unravel the multiple talents of low-valent tin (II). At the molecular level, the interplay between redox-active ligand backbone[1] and tin(II) precursors have led to a series of useful stannylenes[2] and Sn(II) cations.[3] In a handful of cases, the stannylenes showed nucleophilic behavior, while the Sn(II) dications exhibited electrophilic behavior. The redox-active bis(α-iminopyridine) ligand underwent dehydrogenative self-coupling at room temperature in the presence of Sn(II) (*unpublished work*). Using a redox non-innocent ligand system, have led to the synthesis of polystannylene macrocycle with diverse coordinating abilities at the Sn(II) sites.[4] At the nano regime, we have prepared tin/graphenic nano-composites. Tin is known to form several intermetallic phases with Li, however undergoes large volumetric expansion and often exhibit instability with organic electrolytes. Therefore, a composite of tin nanocrystals and carbon nano-sheets has been prepared for application as anode material in lithium ion battery (*unpublished work*).

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4. Manuscript Under Preparation

Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Moumita Majumdar obtained her PhD in 2010 from IIT Kanpur for her research on Transition Metal Multiply Bonded Systems. Subsequently, she joined as Assistant Professor (specially appointed) in Osaka University, Japan where she has worked on Metal Clusters Catalysis. She has gained her expertise in Main Group Chemistry in her Post-Doctoral stint (2011-2014) at the Saarland University, Germany, before joining IISER Pune in October 2014. Her research interest lies in **Main Group Organometallic Chemistry and Materials**.

Cp*Ir(III)-Catalyzed Mild C–H Functionalization of Sulfoximines and Salicylaldehydes

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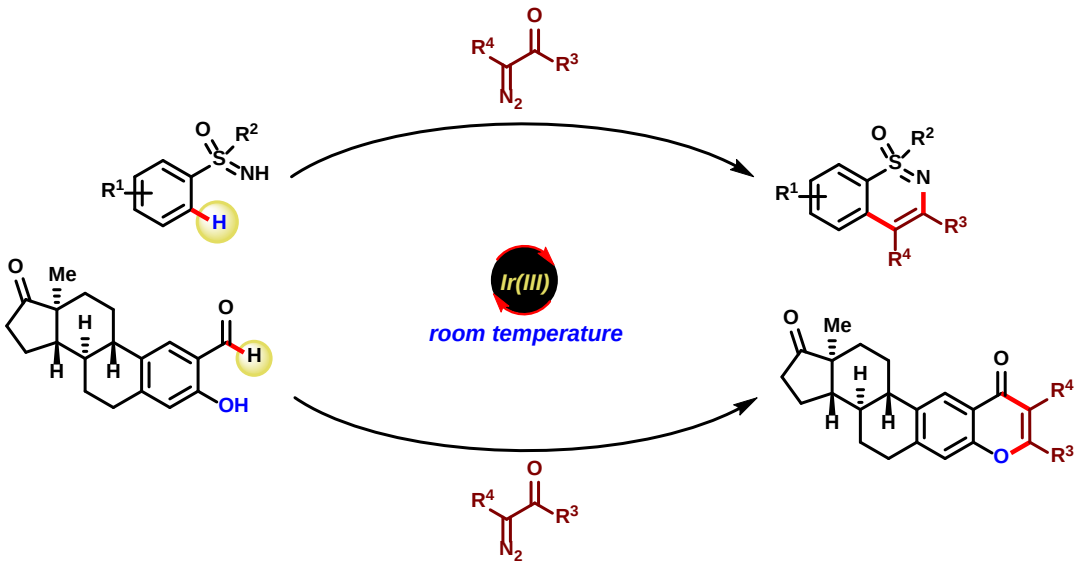
Abstract:
In recent years, the area of mild C−H activation has gained significant importance, as it allows to carry out the reactions at or below room temperature and in the absence of any oxidant or reductant. This results in the enhancement of the functional group tolerance of the reactions, and ultimately leads to the application in the late-stage functionalization of complex biomolecules. Recently, we have reported the first Ir(III)-catalyzed C–H functionalization of sulfoximines with α-diazocarbonyl compounds for the synthesis of 1,2-benzothiazines at room temperature under silver free conditions. We have also utilized a similar catalytic system for C−H/O−H-bond functionalization of salicylaldehydes with α-diazocarbonyl compounds for the synthesis of chromones at room temperature and successfully applied for the late-stage functionalization.

Figure:



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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Dr. Amit B. Pawar completed his M.Sc in Organic Chemistry from University of Pune in 2007. He obtained Ph.D from Indian Institute of Science, Bangalore under the supervision of Prof. Kavirayani. R. Prasad in 2012. He has awarded 1st prize from Eli-Lily for "2012 Lilly Asia Outstanding Thesis Award." He carried out his post-doctoral work with Prof. Sukbok Chang at KAIST, South Korea in the area of C–H bond functionalizations (2013-2015). Later on, he worked as a DST-Inspire Faculty at CSIR-IICT, Hyderabad from April 2015-October 2019. Currently, he is working as an Assistant Professor in the School of Basic Sciences at IIT Mandi, Himachal Pradesh, India. His research is focused on the utilization of first-row transition metals for C–H functionalization and development of mild C–H activation reactions.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Transition Metal Catalyzed α-Heterofunctionalization of Aliphatic Carboxylic Acid Equivalents

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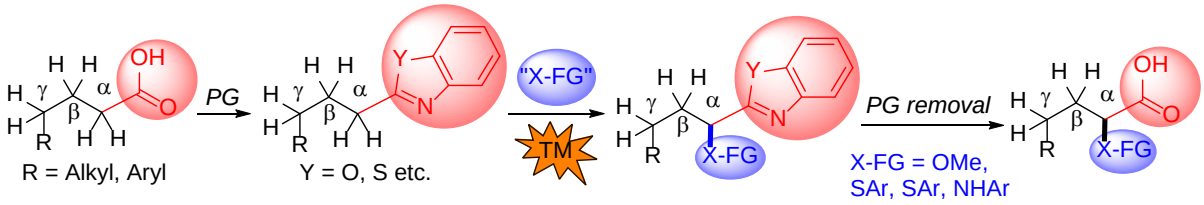
Abstract:
The direct functionalization of unactivated C–H bonds of alkanes has gradually become a thrust area of research in modern organic chemistry for constructing new C–C and C–heteroatom bonds in an atom-economic fashion.[1] Classically, a specific C–H bond of common aliphatic substrates, e.g. carboxylic acids and their synthetic equivalents, is being selectively functionalized based on a directed approach, in which a polar chelating group assists to hold the transition metal catalyst close to the cleavable C−H bond essentially to functionalize β- and/or γ-carbon centers *via* thermodynamically preferred five- or six-membered metallacycle intermediates respectively. However, the functionalization of proximal α-positions with respect to the directing group could not be accomplished *via* directed strategy owing to the prerequisite of a strained four-membered metallacycle intermediate. We have introduced a novel approach that allows the α-functionalization of aliphatic carboxylic acids by transforming them into the corresponding benzazoles.[2] The C(sp^3)–H bonds α-to-the benzazole ring in the 2-alkyl side chain are rather activated by the azole ring presumably due to rapid tautomerization of these systems thereby expediting the required metal catalyzed functionalization process. Relying on this strategy, we have achieved various C–heteroatom bond forming reactions giving expedient access to α-methoxylated (C–O), α-chalcogenated (C–SAr, C–SeAr) and α-aminated (C–NHAr) aliphatic carboxylic acids *via* benzazole intermediates (Scheme 1).



Scheme 1. α-Functionalization of Aliphatic Carboxylic Acids *via* Benzazoles

References and Notes:

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Sukalyan Bhadra received both B.Sc. and M. Sc. degrees in Chemistry from the University of Calcutta (India). In 2011, he was awarded a Ph.D. under the supervision of Professor Brindaban C. Ranu at Indian Association for the Cultivation of Science (India). Subsequently, he moved to Germany, in the group of Professor Lukas J. Gooßen at TU Kaiserslautern for his postdoctoral research. Later in 2013, he joined the group of Professor Hisashi Yamamoto at Chubu University (Japan) as a JSPS postdoctoral fellow. In May 2016, he returned to India and joined CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar, where he currently works as a Senior Scientist. He is intrigued in developing novel methods for metal-promoted organic transformations, cooperative catalysis and asymmetric catalysis towards the synthesis of fine chemicals and API molecules.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Tandem Catalysis Utilizing Methanol

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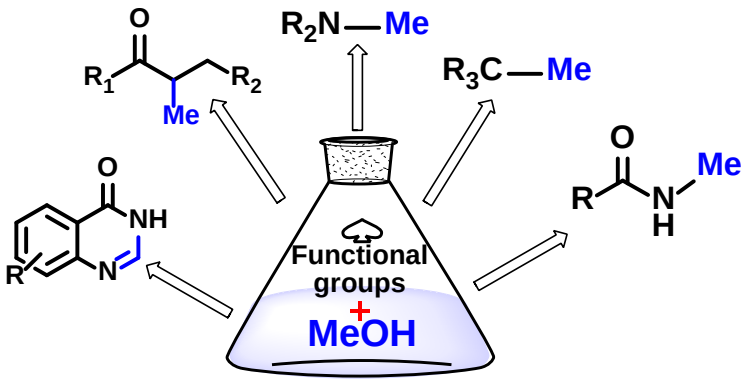
For synthesis of various functionalized molecules utilization of readily available methanol as a C_1 building block is indisputably atom economical and greener strategy compare to the conventional methods. Employing methanol for the first time we reported a simple air and moisture stable Ru(II) catalysed tandem transformation of various nitro compounds and nitriles to the corresponding N-methylated amines.[1,2] We also reported tandem synthesis of α-branched methylated ketones via multicomponent reaction using methanol.[3] Notably, several N,N-dimethyl and N-monomethyl amines were synthesized selectively from organic azides using methanol.[4] This methodology was successfully applied for the one-pot reaction of bromide derivatives with sodium azide. Remarkably, cobalt catalysed tandem conversion of nitrile to N-methylated amide using water/methanol also achieved.[5] Recently, we also reported tandem transformation of aldoximes to N-methylated amides and synthesis of quinazolinone scaffolds using methanol.[6-8] Practical application aspects and mechanistic investigation of these catalytic systems will be presented.



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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Sabuj Kundu obtained his PhD in 2009 from Rutgers, The State University of New Jersey, USA under the supervision of Professor Alan S. Goldman. He worked as a postdoctoral fellow with Professor William D. Jones at University of Rochester, NY (2009-11) and Professor Maurice Brookhart at University of North Carolina at Chapel Hill (2011-13). Subsequently, in 2013 he returned to India to join as an Assistant Professor at the Department of Chemistry, Indian Institute of Technology Kanpur, where he is presently an Associate Professor. He received the DST-INSPIRE Faculty fellowship, India. From IIT Kanpur, he also received P. K. Kelkar research fellowship. His group is focused on various aspects of homogeneous and heterogeneous catalysis for sustainable chemical transformations.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Molecular Diversity through Cascade C-H Activation

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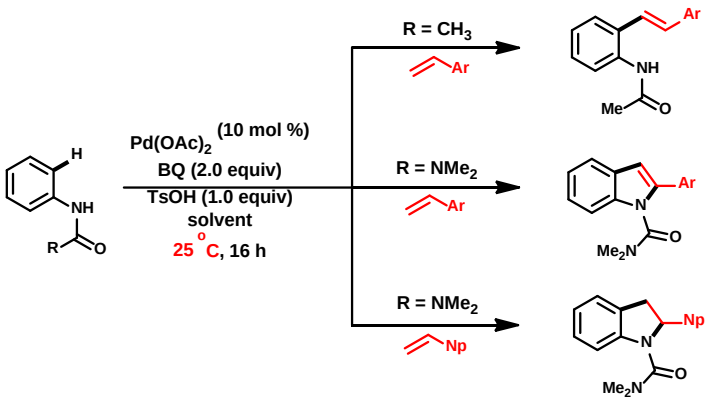
Abstract:
The beginning of the twenty-first century has witnessed significant advances in the field of C–H bond activation, and this transformation is now an established piece in the synthetic chemists' toolbox.[1] This technique is extremely useful for the efficient construction and late-stage labelling of complex natural products or molecules containing multiple stereocenters. Furthermore, this approach has enormous implications for the discovery of small molecules with desired properties, such as catalysts, synthetic reagents, biological probes and new drugs.

In this vein, we are working on the synthesis of structurally diverse medicinal scaffolds via cascade C-H activations. For example, we have accomplished the diversified synthesis of Fujiwara-Moritani Heck product, indole and indolines from aniline derivatives via C-H activation.[2] We have also achieved π-extension to construct dibenzofused carbazoles from indoles through triple C-H activation.[3] We have developed late-stage γ-C-H activation strategy for the synthesis of unnatural amino acids.[4] Furthermore, ortho C-H arylation of inexpensive aniline derivative led to the concise synthesis of Boscalid an agrochemical and Mahanine a carbazole alkaloids. Recently, we have developed a green protocol for the C-H amination in water[5] and carboxylation reaction using carbon dioxide.[6]

Scheme. Diversity oriented synthesis through C-H activation



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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Dr. Ranjan Jana has earned his Ph.D. degree in Organic Chemistry from Indian Association for the Cultivation of Science (IACS) under the supervision of Professor Brindaban C. Ranu. He did his first postdoctoral studies with Prof. Samuel Braverman at Bar-Ilan University, Israel in 2007. Subsequently, he worked with Jon A. Tunge at the University of Kansas, USA where he has developed a green catalyst called “Janaphos” following his name. Next, he joined in the Matthew S. Sigman group at the University of Utah. He returned to India as senior scientist at Organic and Medicinal Chemistry Division, CSIR-Indian Institute of Chemical Biology in 2013. Presently, he is a principal Scientist and adjunct faculty of National Institute of Pharmaceutical Education and Research (NIPER), Kolkata. His field of research includes development of green catalysts, novel synthetic methodology in decarboxylative cross-couplings, C-H functionalization and carboxylation reactions, natural product synthesis and development of bioconjugation techniques.

Awards:

1. Ramanujan Fellowship, SERB, DST, Govt. of India.
2. CSIR-outstanding Scientist, CSIR, Govt. of India.

Manganese Catalyzed Acceptorless Dehydrogenative Coupling and Hydrogen-Auto-Transfer Enables the Stereoselective Synthesis of Alicyclic Compounds

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Abstract:
Multi-substituted alicyclic compounds particularly cyclopentanes, cyclohexanes, and cycloheptanes are omnipresent as the core structure in a wide range of pharmaceutical agents, natural products, and materials. Despite the substantial importance of these multifaceted structural motifs, their modular synthetic routes are limited. Multi-step protocols such as cycloaddition followed by re-duction, cyclodimerization of cyclopropane, ring expansion of cyclopentanone, hydrogenation of aromatic compounds, cyclization of dihalides with methylene nucleophile were traditionally applied for the synthesis of cycloalkanes. All these state-of-the-art approaches count on the dedicated multistep synthesis of the appropriately substituted precursor for a class of compound, and suffers from drawbacks spanning to limited substrate scope, poor regio- or stereoselectivity, or the generation of a stoichiometric chemical waste. Henceforth, an alternative general strategy towards these versatile structural motifs from abundant building blocks is in high demand.
In this report, we showcase a novel bench-stable manganese catalyst that served as an efficient catalyst for the stereoselective synthesis of these important structural units from plentiful building blocks. Large availability and bench stability of the starting precursors would ideally make this process attractive and will allow the uniform synthesis of different families of cycloalkanes with the formation of two moles of water as the sole byproduct.

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3. Maji et al. **2019**, unpublished.

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Biplab Maji, born in Howrah, India, in 1987, obtained his M.Sc. in chemistry from the Indian Institute of Technology Kanpur in 2009. Subsequently he joined the group of Prof. Herbert Mayr at the Ludwig Maximillan Universität Munich for his doctoral studies, which he completed in 2012. In 2013, he joined the group of Prof. Hisashi Yamamoto at the Molecular Catalyst Research Center under Chubu University in Japan as a postdoctoral fellow. In 2015, he joins the group of Prof. Frank Glorius at Westfälische Wilhelms-Universität Münster, Germany as an Alexander von Humboldt fellow. Since 2016, he is working as an assistant professor in the Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata (IISER Kolkata). His research focuses on organic synthesis, catalysis, and mechanistic studies.

Non-Precious Metal-Catalyzed Oxidant Free (De)-hydrogenation of Alcohols

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Abstract:
Amines, amides and N-heterocycles are most valuable compounds ubiquitous in bioactive molecules, alkaloids, and extensively used in pharmaceuticals, agrochemicals and as ligands.[1] Therefore, catalytic selective C–N and C-C bond formation for their synthesis is an ultimate goal in chemical research. Conventional methodologies for their synthesis involves multi-step pathways and suffer from low atom economy, limited selectivity and produced stoichiometric amounts of waste.[1] Direct application of renewable alcohols as electrophilic coupling partner represents a sustainable alternative, as they can be readily available in industrial scale production from lignocellulose biomass.[1]
Recently, there is a potential drive to replace the precious noble-metal catalysts using earth abundant and inexpensive non-noble metals for sustainable organic transformations. We have developed the applications of Ni-based catalysts for such transformations. We have studied a general and practical applications of various primary alcohols, including diols and amino alcohols for selective construction of various primary and secondary amines, amides, five or six-membered N-heterocycles, activation of weak sp^3 C-H bond of alkyl substituted heteroarenes to *E*-selective alkenes as well as functionalization of ketone enolates. A detailed mechanistic and kinetics studies were also established for such transformations.[2-8]

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8. Das, J.; Vellakkaran, M.; Sk. M.; Banerjee, D. *Org. Lett*., **2019** *21*, 7514-7518.

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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Debasis Banerjee graduated with M.Sc. degree in Organic Chemistry from Banaras Hindu University and obtained Ph.D. in organic chemistry from Indian Institute of Technology Kanpur in 2011 with Prof. M. L. N. Rao. Thereafter he moved to Leibniz Institute for Catalysis (LIKAT), Germany for a postdoctoral position with Prof. Matthias Beller (2011-14) and subsequently held another postdoctoral position (2014-2015) at the Stockholm University, Sweden with Prof. Jan-Erling Bäckvall. Currently he is an Assistant Professor at Indian Institute of Technology Roorkee from March 2015. His research interests include design and synthesis of sustainable catalysts, enantioselective dual-catalysis, activation of small molecules, activation and functionalization of sp^3 C-H bond and heterogeneous catalysis for sustainable organic transformations. He is a recipient of SERB-Early Career Research Award (2016), DAE-Young Scientist Research Award (YSRA-2016) and winner of Evonik Call for Research Proposal (ECRP-2016) Award by Evonik Industries GMBH, Germany. Recently he has received Thieme Chemistry Journals Award 2020.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Catalytic Cross-Coupling of Secondary Alcohol

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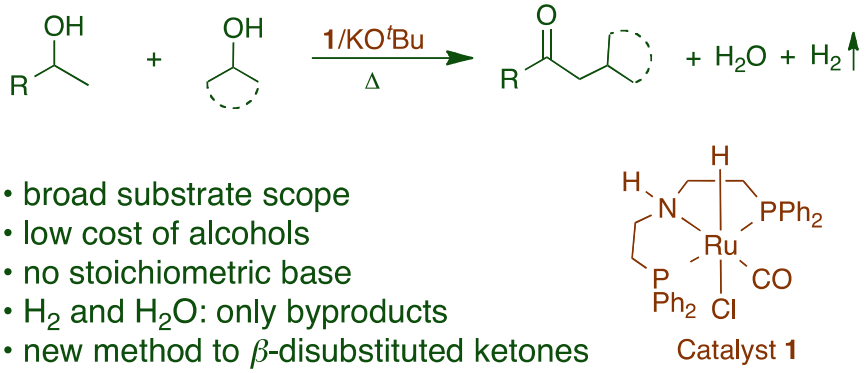
Abstract:
An unprecedented ruthenium(II) catalyzed direct cross-coupling of two different secondary alcohols to *β*-disubstituted ketones is reported. Cyclic, acylic, symmetrical, and unsymmetrical secondary alcohols are selectively coupled with aromatic benzylic secondary alcohols to provide ketone products. A single catalyst oxidizes both secondary alcohols to provide selectively *β*-disubstituted ketones to broaden the scope of this catalytic protocol. Number of bond activation and bond formation reactions occur in selective sequence via amine-amide metal-ligand cooperation operative in Ru-MACHO catalyst. The product-induced diastereoselectivity was also observed. Kinetic and deuterium labeling experiments suggested that the aliphatic secondary alcohols undergo oxidation reaction faster than benzylic secondary alcohols, selectively assimilating to provide the cross-coupled products. Reactions are sensitive to steric hindrance. This new C□C bond forming methodology requires low catalyst load and catalytic amount of base. Notably, the reaction produces H_2 and H_2O as the only by-products making the protocol greener, atom economical and environmentally benign



Scheme 1. Ruthenium-Catalyzed Cross-Coupling of Two Different Secondary Alcohols

References and Notes:

1. Thiyagarajan, S.; Gunanathan, C. *J. Am. Chem. Soc.* **2019**, *141*, 3822-3827.
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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Professional Experience

2017- Associate Professor, NISER Bhubaneswar, India
2013- Reader F, NISER Bhubaneswar, India
2011- Assistant Professor, NISER Bhubaneswar, India
2011- Ramanujan Fellow (SERB), NISER Bhubaneswar, India
2009- 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, Bhavnagar, India
1999 M. Sc Department of Organic Chemistry, University of Madras, India
1997 B. Sc RKM Vivekananda College, University of Madras, India

Awards

Thieme Chemistry Journals Award 2020
Selected for CRSI Bronze medal 2020
Top Peer Reviewer Award 2019 by Publons
ECRP award 2016 -First Prize (10,000 Euro).
Ramanujan Fellowship (Sept. 2011-Aug. 2016). SERB, New Delhi.
AvH Research Fellowship (2009- 2011). RWTH Aachen University, Germany.
Dean of Faculty Postdoctoral Fellowship (2006-2008) by Weizmann Institute of Science, Israel.

Research Interests: *Catalysis*
Organometallic Chemistry
Reaction mechanism, and Synthetic methods.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Metal-free Synthesis of Trifluoromethylated Heterocycles Employing Trifluorodiazoethane

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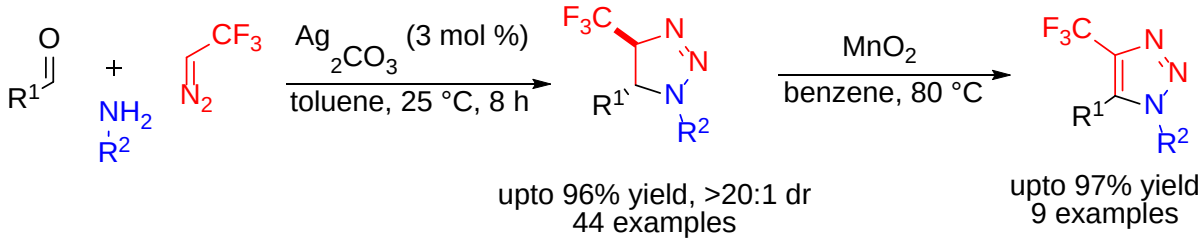
Abstract:
The incorporation of the trifluoromethyl group can significantly improve the physicochemical and biological properties of the compounds, such as catabolic stability, bioavailability, and lipophilicity. In this context, trifluorodiazoethane, a fascinating small molecule reagent, has recently emerged as a versatile reagent for the synthesis of valuable CF_3-containing subunits. Mykhailiuk and Ma groups reported [3+2] cycloaddition reactions for the synthesis of CF_3-substituted pyrazolines and pyrazoles by using electron-deficient olefins with CF_3CHN_2.[1] Molander and co-workers reported a facile synthesis of CF_3-substituted isoxazolidines through the three-component reaction of CF_3CHN_2 with nitrosoarenes and alkenes.[2] It may be noted that 1,2,3-triazolines are important structural motifs with widespread use in medicinal chemistry, and to our knowledge, CF_3CHN_2 has not been applied for the synthesis of such important scaffolds bearing trifluoromethyl moiety. Recently, a three-component domino reaction involving aldehydes, aliphatic amines, and CF_3CHN_2 has been uncovered for the diastereoselective synthesis of 1,2,3-triazolines.[3] This step and atom-economic protocol requires only a very low catalyst loading, displays a broad substrate scope with good functional group tolerance, and provides good to excellent yields with high diastereoselectivities.



Scheme: Synthesis of trifluoromethylated 1,2,3-triazolines

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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Kishor Mohanan is a Principal Scientist in the Division of Medicinal and Process Chemistry at CSIR-Central Drug Research Institute, Lucknow. He obtained his PhD degree in chemistry in 2007 under the guidance of Dr. Vijay Nair from CSIR-National Institute for Interdisciplinary Science and Technology, Trivandrum. Subsequently, he worked as a post-doctoral fellow in the research groups of Prof. B.-J. Uang at National Tsing Hua University, Taiwan, Prof. Michael Smietana at University of Montpellier, and Prof. Jean Rodriguez at Aix-Marseille University, France, before joining CSIR-Central Drug Research Institute in 2013 as a Senior Scientist. His current research focuses on the development of new reactions employing diazo compounds for the synthesis of medicinally relevant heterocycles.

Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

Bifunctional Organocatalytic Michael Additions as the Key Strategy: Enantioselective Synthesis of Fused and Spirocyclic Organic Molecules

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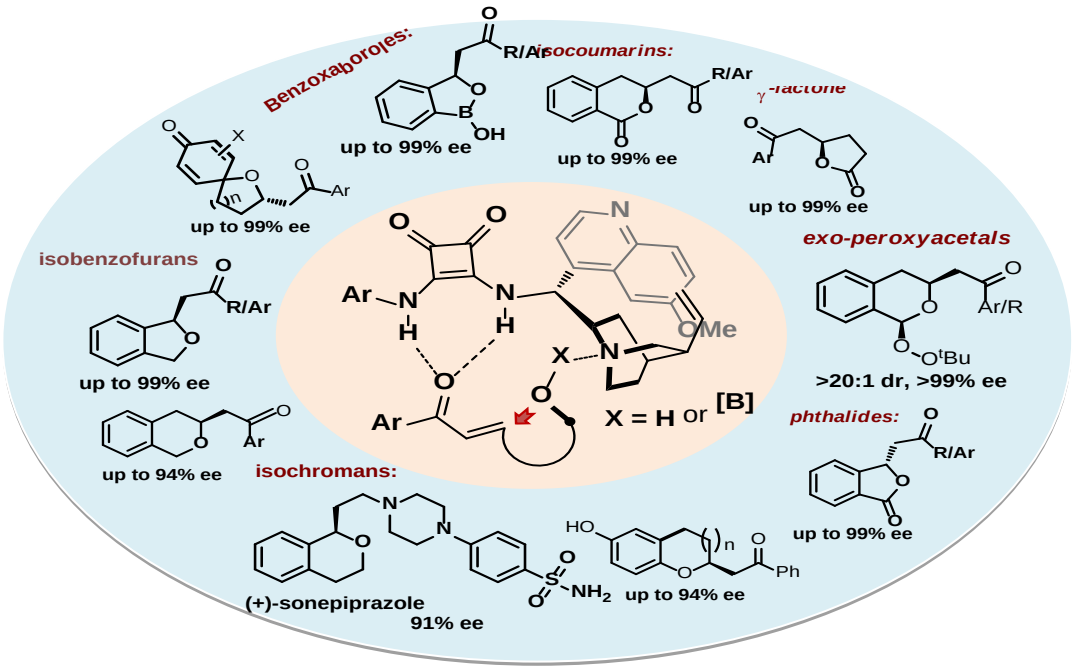
Abstract

Intramolecular oxa-, aza- and carba-Michael reactions are the most fundamental but very powerful tools to construct oxa-, aza-, and carba-cycles, respectively. The development of the corresponding asymmetric variants, often, remained significantly challenging.[1] We have developed few independent cinchona alkaloid based chiral bifunctional amino-thiourea/ squaramide catalyzed strategies for efficient enantioselective cyclization of alcohol, emnamine, and carbon nucleophiles for the synthesis of chiral oxa-, aza-, and carba-cycles, respectively.[2-5]



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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Prasanta Ghorai obtained his B.Sc. (Hons in Chemistry) from Vidyasagar University, West Bengal. Subsequently, he did his M.Sc. (Chemistry) from IIT Bombay in 2002 and Ph.D. at the University of Regensburg, Germany in the area of Organic and Medicinal Chemistry in 2005. Afterward, he was involved in post-doctoral research at the University of Nebraska-Lincoln in USA from 2005-2009. He joined the then new IISER Bhopal as an Assistant Professor (Chemistry) in 2009 and became Professor in 2019. He is honoured as DAAD Research Ambassador of India by DAAD Germany. Dr. Ghorai has been selected for the prestigious Chemical Research Society of India (CRSI) Bronze Medal for the year 2017 for his contribution in Chemistry.

Dr. Ghorai's research work falls in the area of synthetic organic chemistry, more specifically, asymmetric synthesis and catalysis. The main aim of his group is to develop new strategies and chiral catalysts for enantioselective reactions.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Catalyst-Controlled Remote Para Selective C–H Bond Activation and Borylation of Aromatic Amides

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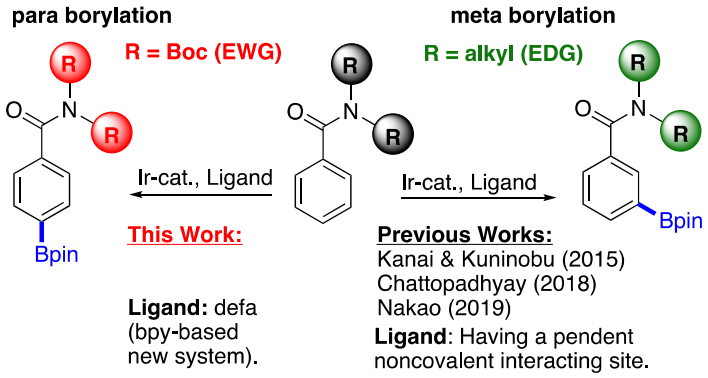
Abstract:
The selective activation of remote para C–H bonds of arenes is highly challenging employing transition metal catalysis. While iridium-catalyzed C–H activation and borylation has appeared as the leading technology for the arene borylation, there are very few methods for the remote para borylation. We have developed an efficient strategy, which affords remarkably high para selectivity of aromatic amides. For achieving high para selectivity, a new catalyst system has been engineered using Ir-metal and defa ligand. Moreover, it has also been demonstrated in the present studies that substrate's geometry also plays an important role for high level of remote para selectivity. We hypothesis that the origin of selectivity is due to the geometric constrains of the newly engineered catalyst system employing defa ligand (in-plane distortion occurs owing to the intervening methylene group) and bis-Boc amides (fully twisted geometry). The details will be presented in the conference.[1]



References and Notes:

1. Hoque, E.; Bisht, R.; Chattopadhyay, B. (Unpublished results).

Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Buddhadeb graduated (2003) with M.Sc. in Organic Chemistry from Visva-Bharati University (Santiniketan) and earned Ph.D. degree in Synthetic Organic Chemistry from the University of Kalyani (2009), West Bengal. In 2009, he accepted a postdoctoral research associateship from the University of Illinois at Chicago, USA in the group of Professor Vladimir Gevorgyan. Spending two years at Chicago, he then moved to the Michigan State University, Michigan, USA for his next postdoctoral research program in the laboratories of Professor Milton R. Smith III. Group (2011-July 2014). In August 2014, he moved to the Centre of Biomedical Research (CBMR) Lucknow, India as a DST-Ramanujan Faculty and since November 2016, he is working as an Assistant Professor. His research interest includes design and synthesis of new catalytic systems employing various noncovalent interactions for the C–H bond activation/borylation/silylation and synthesis of medicinally important heterocyclic molecules via metal-nitrene/carbene chemistry. Buddhadeb is a recipient of Thieme Chemistry Journal Award (2017), DST-Young Scientist Award (2015), and DST-Ramanujan Fellowship (2014).

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

CO_2 Conversion Catalysis: Toward Sustainability

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Abstract:
"Methanol Economy" and *"Hydrogen Economy"* have been proposed as potential solution for much-demanding carbon-neutral energy cycle. Chemical hydrogen storage (CHS) within CO_2 through catalytic hydrogenation and as-required delivery of hydrogen through a reverse catalytic dehydrogenation process is an interesting concept in this context. However, a sustainable catalytic protocol is the primary requirement in this prospective technology. One major research program in our laboratory is focused on this issue.
With the help of recently-developed *"Switchable Catalysis"* approach,[1] we have demonstrated our initial efforts in this area by devising an ambient-pressure H_2-storage and low-temperature H_2-release with CO_2/HCO_2H couple catalysed by a pH-responsive "Ir-NHC" complex.[2] The developed concept triggered to discover the first ever atmospheric-pressure CO_2-conversion strategy which does not require H_2 gas and instead uses renewable hydride donors.[3] The later approach is currently being upgraded in our laboratory to achieve a sustainable CO_2-conversion protocol. This poster will highlight the above findings.

References and Notes:

1. (a) Semwal, S.; Choudhury, J. *ACS Catal.* **2016**, *6*, 2424−2428; (b) Semwal, S.; Choudhury, J. *Angew. Chem. Int. Ed.* **2017**, *56*, 5556–5560, and https://www.chemistryworld.com/news/ruthenium-complex-catalyses-complimentary-reactions/3007136.article; (c) Maji, B.; Choudhury, J. *Chem. Commun.* **2019**, *55*, 4574–4577.
2. Semwal, S.; Kumar, A.; Choudhury, J. *Catal. Sci. Technol.* **2018**, *8*, 6137–6142.
3. Kumar, A.; Semwal, S.; Choudhury, J. *ACS Catal.* **2019**, *9*, 2164–2168; and https://www.chemistryworld.com/news/taking-the-pressure-off-catalytic-carbon-dioxide-conversion-/3010094.article.

Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Joyanta Choudhury obtained Ph.D. in 2006 from IIT Kharagpur, India working under Professor Sujit Roy on the development of well-defined 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 alkane functionalization (CH_4-to-CH_3OH) 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 coordination-driven molecular assemblies on solid surfaces. Currently, he is an Associate Professor at the Department of Chemistry, IISER Bhopal, India. His research focusses on (a) developing new reactivity with metal-NHC complexes, (b) small molecule activation-functionalization including CO_2, H_2, alkanes, arenes, and H_2O, and (c) developing switchable organometallic catalysts to address renewable energy related problems. His research works on '*Switchable Catalysis*' and '*CO_2-conversion Chemistry*' have been covered as News in the popular RSC magazine, *ChemistryWorld*. He has been featured as '*Movers & Shakers*' by the industry-leading magazine '*The Catalyst Review*', published by The Catalyst Group (TCG), PA, USA. He has been awarded with the Bronze Medal of the Chemical Research Society of India (CRSI) for the year 2019. From 2020, he is a member of the Editorial Advisory Board (EAB) of *ACS Catalysis*.

Metal-Catalyzed Alkyne Annulation Reactions for the Synthesis of Important Heterocycles

Sanjib Gogoi*

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Abstract:

In last few decades, the transition-metal-catalyzed C−H bond activation, followed by alkyne annulation reactions have emerged as excellent methods for the efficient synthesis of various important heteroaromatic compounds, which are otherwise difficult to be synthesized by using conventional synthetic methods.[1] We have been working on the development of novel metal-catalyzed reactions for the synthesis of various heterocycles.[2] Very recently, we have developed novel methods for the synthesis of heterocycles such as pentafulvenes, spiro-benzofuranones, spiro-pyrazolones, bis(spiro-pyrazolones), indolo[2,1-*a*]isoquinolines, pyrimidoindolones etc., using metal-catalyzed C-H activation and alkyne annulation as the key reaction. These reactions will be presented briefly in the symposium.

References:

1. Gandeepan, P.; Müller, T.; Zell, D.; Cera, G.; Warratz, S.; Ackermann, L. *Chem. Rev.* **2019**, *119*, 2192-2452.
2. (a) Borthakur, S.; Baruah, S.; Sarma, B.; Gogoi, S. *Org. Lett.* **2019**, *21*, 2768-2771. (b) Borthakur, S.; Sarma, B.; Gogoi, S. *Org. Lett.* **2019**, *21*, 7878-7882. (c) Phukon, J.; Gogoi, S. *Chem. Commun.* 2019, DOI: 10.1039/C9CC09564K.

Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Education:

- Ph. D., Organic Chemistry, 2008, National Chemical laboratory, Pune, India (Pune University)
- M. Sc., Organic Chemistry, 2001, Dibrugarh University, Dibrugarh, Assam, India
- B. Sc., Chemistry, 1998, DHSK College, Dibrugarh University, Dibrugarh, Assam, India

Professional Experience:

- Senior Scientist, CSIR-NEIST, Jorhat-785006, Assam, India, Oct 2015-Till date
- Scientist, CSIR-NEIST, Jorhat-785006, Assam, India, Oct 2011-Oct 2015
- Postdoctoral Fellow, Wayne State University, Detroit, Michigan, USA, 2009-2011
- Postdoctoral Researcher, University of Texas at San Antonio, San Antonio, Texas, USA, 2008-2009

Awards and Honors:

- Chemical Research Society of India (CRSI) Bronze Medal, 2019
- Thieme Chemistry Journal Award, 2019
- Professor D. K. Banerjee Memorial Lecture Award, Department of Organic Chemistry, IISc.,
- Bangalore, 2018
- DST-SERB Fast Track Project Award, 2015
- Senior Research Fellowship (SRF), CSIR, 2004-2007
- Junior Research Fellowship (JRF), CSIR, 2003-2004
- Ranked first in M.Sc. (Organic Chemistry) of 1999-2001, Dibrugarh University

Research Interests

- Development of novel metal-catalyzed reactions
- New process development for valuable compounds
- Total synthesis of bioactive natural products and natural product hybrids

Hantzsch Ester as Photo-Organocatalyst under Visible Light Irradiation

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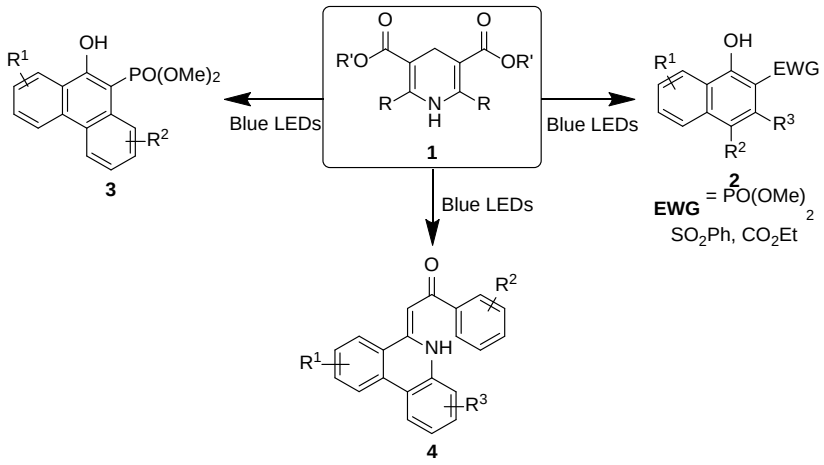
Abstract:
In the last decade, the visible light photoredox catalysis has witnessed tremendous growth in terms of novel organic transformations including C-C as well as C-X (X = halogens, B, O, P, S, Se) bond forming reactions.[1] The visible light mediated reactions usually employ organic dyes or metal-polypyridyl complexes as photocatalysts. Since the use of metal photocatalysts defeats the very objective of developing "greener" reactions under visible light irradiation, the development of novel organic photocatalysts is highly desired. In this context, several organic molecules such as benzophenones, acridinium salts, pyrilium salts, phenylglyoxalic acids, Hantzsch esters etc. have been employed as photo-organocatalysts for the visible light promoted rections.[2]

The Hantzsch esters **1** are efficient single electron as well as hydrogen atom donors upon visible light irradiation and can mediate photoredox reactions with or without another photocatalyst. In this presentation, our group's results on visible light mediated synthesis of valuable carbocycles/heterocycles such as naphthalene-1-ols **2**, phenanthrene-1-ols **3** and phenanthridine chalcones **4** employing Hantzsch ester as photo-organocatalyst will be discussed.[3]



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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis(ICOC 2020)

Bio-Sketch of Speaker

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Namrata Rastogi obtained Ph.D. in synthetic organic chemistry from Indian Institute of Technology, Bombay in 2006. She worked as postdoctoral research associate at the Indian Institute of Technology, Kanpur and University of Minnesota, Minneapolis, USA, during 2006 to 2009. She then served as research scientist in Jubilant Biosys Drug Discovery and Development, Bengaluru, Karnataka for 2 years before joining CSIR-Central Drug Research Institute, Lucknow in 2011.

Her research interests include exploring novel visible light photoredox catalyzed organic transformations and developing new photocatalysts. Her research group is also involved in the CSIR-CDRI's drug discovery program in the area of parasitic diseases, developing small molecules against Leishmania and Malaria parasite particularly.

Namrata Rastogi served as INSA-DFG visiting faculty in the University of Regensburg, Germany in 2014. She is a recipient of Indian Society of Chemists and Biologists (ISCB) Distinguished Women Scientist Award-2019 in the area of Chemical Sciences.

2,2′-bibenzimidazole based Ruthenium(II)-Para-Cymene: Robust Metal-Ligand Bifunctional Catalyst for Chemo Selective reduction of α,β-Unsaturated Carbonyl

Manali Dutta,[a] Subhamoy Mukhopadhyay,[a] and Sanjay Pratihar*[,a,b]
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Abstract:
Nature uses smart biological machines (SBM) for carrying out uncountable parallel processes without interfering with one another with an unimaginable level of control. In order to mimic such smart activity by artificial catalysts for different chemical transformations remain scarce [1-2]. However, in past few years, few SBMs have been developed through the incorporation of reversibly stimuli responsive, function regulatory feature(s) utilizing various external stimuli, including acid−base, mechanical force, redox processes, and light to modulate the intrinsic activities and/or selectivity displayed by these catalysts [3-7]. Herein, we disclosed the complex of BiBzImH2 with Ru(II) para cymene (**C-1**, containing imino-type σ-donating N→Ru coordination) for its proton and substrate responsive switchable function between its anionic state (**C-2**, containing anionic σ- and π-donating amido-type N–Ru covalent bonding) for their utilization as stimuli (base/acid) or substrate (α,β-unsaturated carbonyl) responsive function for chemo selective reduction of α,β-unsaturated carbonyl to corresponding saturated carbonyl [8]. The chemo selective reduction of α,β-unsaturated carbonyl to corresponding saturated carbonyl or unsaturated alcohol or saturated alcohol utilizing triethyl silane (Et_3Si-H) or hydrogen balloon as hydrogen source depends upon; (i) the catalyst-substrate interaction through hydrogen bond, (ii) substituent attached on the substrate and catalyst, and (iii) solvent of the reaction. The mechanism of reduction was assessed from spectroscopic, kinetic, and few other controlled experiments and showed its quality performance for variety of substrates with good selectivity and turn over frequency (TOF) with reasonable functional group tolerance.

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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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INSA Young Scientist (2017-2019), Tezpur University, Assam-784028, India.

DST-Inspire Faculty (October, 2012 to October 2017), Tezpur University, Assam-784028.

Awards & Honors

Gandhian Young Technological Innovation (GYTI) Award-2018 at Rastrapati Bhavan, India.

Indian National Science Academy (INSA) Medal for Young Scientist-2017.

Research Area

Mechanistic Organometallic Chemistry and Catalysis.

Catalytic, Photocatalytic and Agricultural Applications of Smart Materials.

Education

Doctor of Philosophy: Department of Chemistry, IIT Kharagpur, India; (07-2006 to 01-2012).

Master of Science: (Inorganic Chemistry), Banaras Hindu University, India, (2004− 2006).

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Ruthenium-Catalyzed Cyclization of Substituted Aromatics or Alkenes with Carbon-Carbon π-Components: an Efficient Route to Heterocycles

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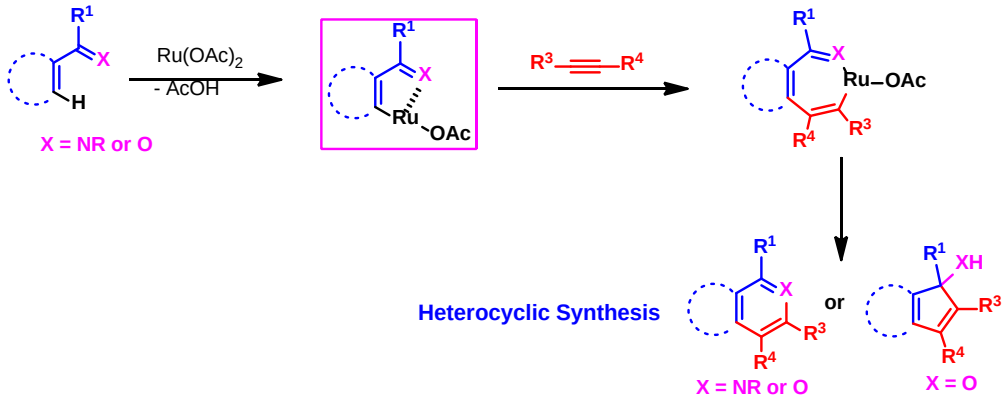
Abstract:
The transition metal-catalyzed chelation-assisted cyclization of heteroatom substituted aromatics with carbon–carbon π-components via chelation-assisted C–H bond activation is one of the promising and practical methods to synthesize carbocyclic and heterocyclic compounds.[1] This type of oxidative cyclization is highly atom-economical and environmentally friendly when compared with the other conventional methods. Palladium, rhodium, cobalt and ruthenium complexes have been widely used as catalysts for this reaction. Among them, a less expensive ruthenium complex has gained tremendous attention recently, due to their remarkable reactivity, compatibility and selectivity.[1] In addition, most of this cyclization reaction can be done under an air atmosphere. Our group has been working in the ruthenium-catalyzed C-H bond functionalization reaction for the past eight years. In this talk, I would like to present our recent observation on cyclization of heteroatom substituted aromatics with carbon-carbon π-components in the presence of a ruthenium catalyst via C-H bond activation reaction.[2] This method provides an efficient route to various heterocyclic molecules such as isocoumarins, indenols, isoquinolines, isoquinolones, α-pyrones, 2-quinolinones and isoindolinones in good to excellent yields.



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Masilmani Jeganmohan was received his master's degree in organic chemistry from the University of Madras in 2001. He earned his PhD from the National Tsing Hua University, Taiwan, under the guidance of Prof. Chien-Hong Cheng in 2005 and pursued postdoctoral work in the same laboratory (2005–2009). Then, he moved to the Ludwig-Maximilians-Universitat, Munich, Germany, for a postdoctoral study with Prof. Paul Knochel supported by Alexander von Humboldt foundation (2009 to 2010). He started his independent research carrier in November 2010 at IISER Pune as an assistant professor. In April 2016, he was promoted to associate professor at IISER Pune. At present, he is working as an associate professor at Indian Institute of Technology Madras (October 2016–till now). He was the recipient of DAE Young Scientist Research Award (2011), Science Academy Medal for a young associate, Indian Academy of Sciences (2012-2015), Science Academy Medal for Young Scientists, Indian National Science Academy (2013), Alkyl Amines – ICT Young Scientist Award by Institute of Chemical Technology Mumbai (2013), ISCB Award of Appreciation for Chemical Science, CSIR-CDRI (2014), India and a Fellow Royal Society of Chemistry (FRSC). His research interest includes the development of new synthetic methods using metal complexes as catalysts, asymmetric synthesis and natural product synthesis.

Design and Synthesis of silver decorated Fe_3O_4 @ Fe doped CeO_2 core @ shell ternary composite as highly efficient nanocatalyst for selective oxidation of alkenes.

Topi Ghosh,[a] Neha Choudhary[a] and **Shaikh M. Mobin***[a,b,c]

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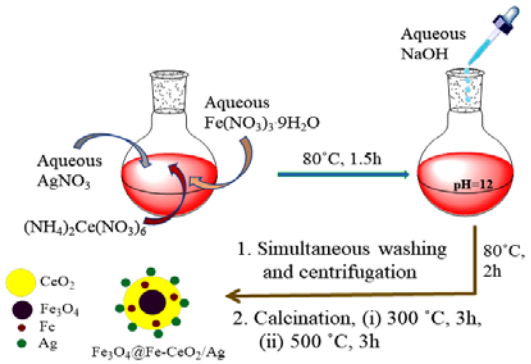
Abstract:
Well define silver decorated Fe_3O_4 @ Fe doped CeO_2 core @ shell ternary composite based nanocatalyst was designed and synthesized. The characterization of prepared nanocatalyst Fe_3O_4@Fe-CeO_2/Ag was carried out by using various techniques such as XRD, HRTEM, SEM-EDAX-mapping, BET, FTIR, TGA and XPS analysis. This Fe_3O_4@Fe-CeO_2/Ag nanocatalyst undergoes alkenes oxidation which showed 100% conversion of styrene with 95% selectivity for benzaldehyde by using 70% aqueous tert-butyl hydroperoxide (TBHP) under optimum reaction condition. The Fe3O4@Fe-CeO2/Ag catalyst was further evaluated for substrate scope showed an excellent conversion, high selectivity for corresponding aldehydes with excellent reusability of catalyst.



Scheme 1. Schematic representation for the synthesis of (Fe_3O_4@Fe-CeO_2/Ag) using co-precipitation method

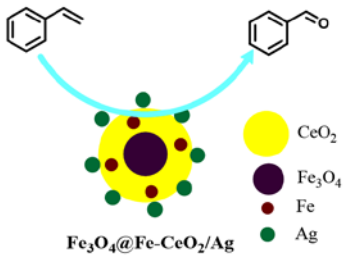


Figure 1: Selective oxidation of alkenes by using Fe_3O_4@Fe-CeO_2/Ag **nanocatalyst.**

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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Dr. Shaikh accomplished his Bachelor's and Master's from Wilson College, University of Mumbai with major in Chemistry and PhD from Mumbai University in Chemistry. In 2012, he joined IIT Indore and presently working as an Associate Professor in Discipline of Chemistry. He had developed his research group working in wide area of research including Optical and electrochemical sensing, Single-Crystal-to-Single-Crystal (SCSC) Transformation, MOFs based Supercapacitors for energy storage, catalysis, sensing and bio-medical applications, metal nano-oxide materials derived by employing metal complexes as single-source molecular precursors as catalyst in organic transformation and greener c-dots. Moreover, the research group designs and synthesizes small molecules as cellular organelles target, cell imaging and docking.

Achievements:

- Dr. Shaikh has been recognised as the Outstanding Reviewers for Dalton Transactions in 2018 (*Dalton Trans.*, 2019, ***48***, 4758-4758).
- Dr. Shaikh has been listed amongst highly prolific authors by ***Current Science***, (*CURRENT SCIENCE, VOL. 109, NO. 5, 10 SEPTEMBER 2015*) rivalling researchers from prestigious institutions such as CSIR-IICT, CSIR-NCL and IIT Kharagpur.
- Recognised among top 10 researchers in Chemistry in India by ***Careers 360*** (Most Outstanding Researcher Award, 2018) with a *h*-index of 44, more than 385 publications and ~7400 citations to date.
- Research work on novel dye for tracking lysosomes in live cell imaging covered by ***Free Press Journal*** Indore edition (April 14, 2018).

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Rhodium–catalyzed Heteroannulation in the Synthesis of Indoles *via* C–H Functionalization and Concomitant Cascade Cyclization

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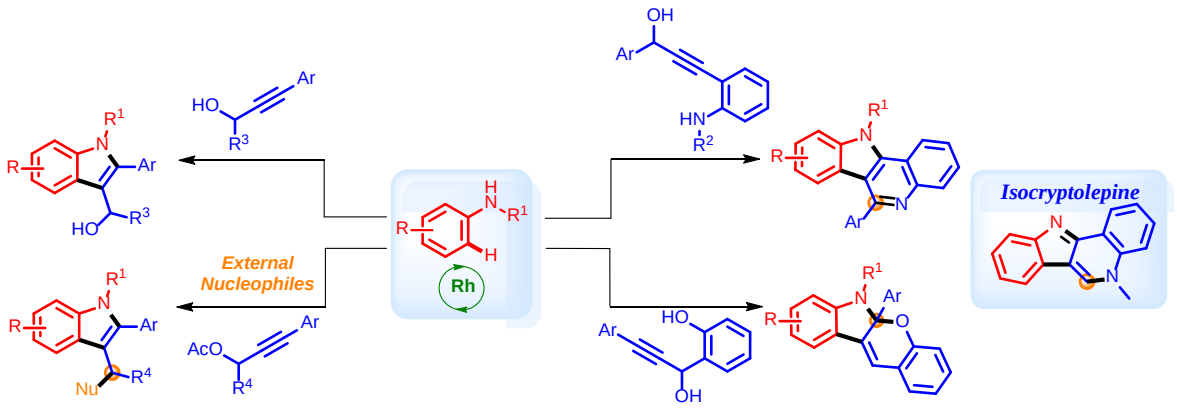
Abstract:
Indole-containing heterocyclic frameworks play a vital role in bioscience, medicine, and chemistry.[1] As one of the most attractive sub-types of indole alkaloids, highly substituted γ-carbolines are the basic structural units in many natural products and pharmaceuticals.[2-3] Herein, we report a rhodium□catalyzed synthesis of □-carbolines, dihydrochromeno[2,3-*b*]indoles, diindolylmethane (DIM) derivatives *via* heteroannulation followed by cascade cyclizations with external and internal nucleophiles.[4] The reaction features highly effective transformations involving two C-C, two C-N and two C-O bonds, leading to the formation of a variety of molecular frameworks which are a part of several biologically active natural products.



Scheme 1

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4. Nagtilak, P. J.; Kapur, M. (*manuscript submitted*).

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Dr. Manmohan Kapur received his Ph.D. degree in 2003, working at the National Chemical Laboratory, Pune. In the same year, he joined the group of Prof. Jin K. Cha at the Wayne State University, Detroit, USA as a postdoctoral fellow. In 2004, he was awarded the Alexander von Humboldt Post-doctoral Research Fellowship for his second postdoctoral position at the Institut für Organische Chemie, Universität Tübingen, Germany, under the guidance of Prof. Martin E. Maier. He joined IISER Bhopal in 2009 and is currently an Associate Professor in the Department of Chemistry. His research interests include the total synthesis of natural products by employing transition-metal catalysis as the key step and synthesis of natural products bearing peptide-based backbones, especially certain classes of anti-mycobacterial agents. He is the recipient of the CRSI Bronze medal 2020 and the SERB-STAR Award 2020.

Flash Talk & Poster Presentation
International Conference on Organometallics and Catalysis (ICOC 2020)

Alkali Metal Mediated Acylation of sp^3 Carbon Centres Using Methyl Esters *via* C-O Bond Cleavage

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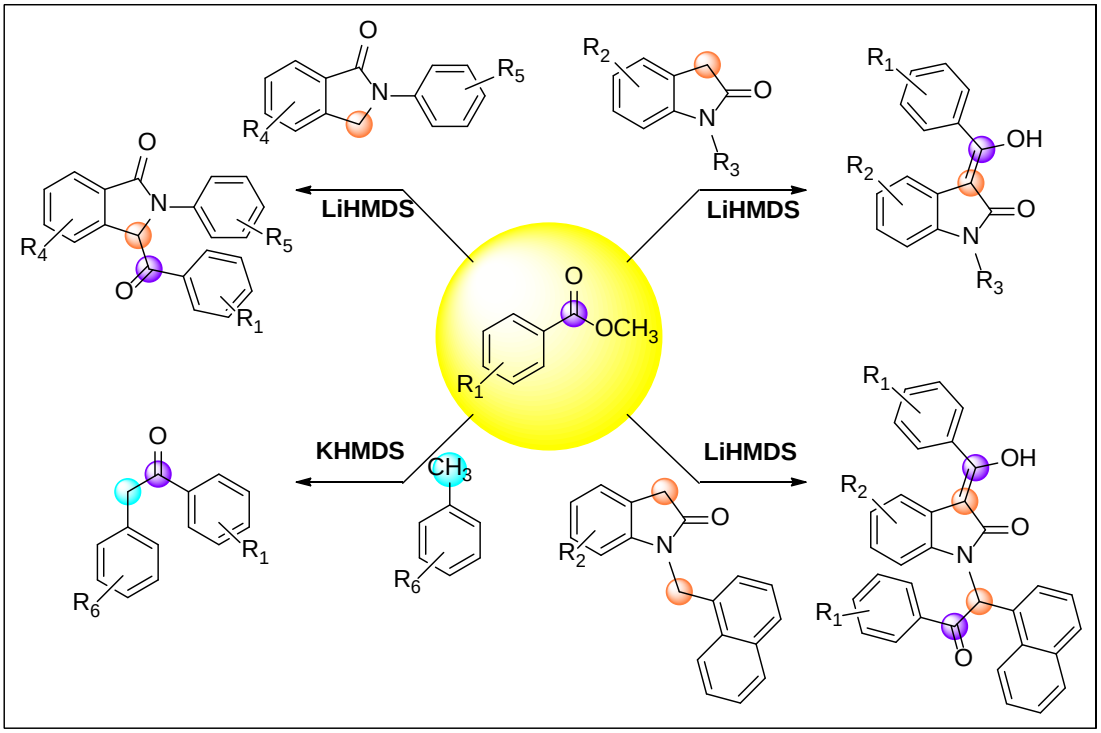
Abstract:
Esters are ubiquitous chemical entity occurs in natural products, pharmaceuticals, and functional materials, and they take a sweet spot on shelves of chemistry laboratories. Owing to their inertness and facile preparation, they were commonly used as solvents and finds vast industrial applications. To counter the inherent robustness of esters and to utilize it, transition metal catalysts, harsh reaction conditions, and organometallic reagents were engaged.[1] Besides, utilization of simple ester, i.e., methyl ester as acyl electrophiles are uncommon.[2] Herein, we unveil a unique alkali metal-mediated acylation of N-substituted 2-oxindoles, isoindolinones, toluene and dual functionalization of N-naphthyl 2-oxindoles using readily available simple methyl esters in the presence of LiHMDS and KHMDS.



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2) a) Hie, L.; Fine Nathel, N. F. ; Hong, X. -F; Yang, Y.; Houk, K. N.; Garg, N. K. *Angew. Chem. Int. Ed.* **2016**, *55*, 2810-2814. b) Zheng, Y.-L.; Newman, S. G. *ACS Catal.* **2019**, *9*, 4426-4433

Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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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 VIT University, Vellore in 2011. His research interests include the development of novel catalysts and its application towards C-H activation/functionalization.

Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

Weak Interactions to Control C-S Bond Formation Reactions

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Abstract:
On the way to weakening of strong chemical bonds *via* weak interactions (soft fore) is significant in both making new chemical systems with functions or to understand the complex functions of living systems. It will be discussed how soft force[1] of several low-energy and low-level interactions or weak interactions are explored to control certain reactivity of chemical systems (Figure 1).Various aspects of metal free C-S bond formation reactions controlled by weak interactions will be discussed.[2-5]

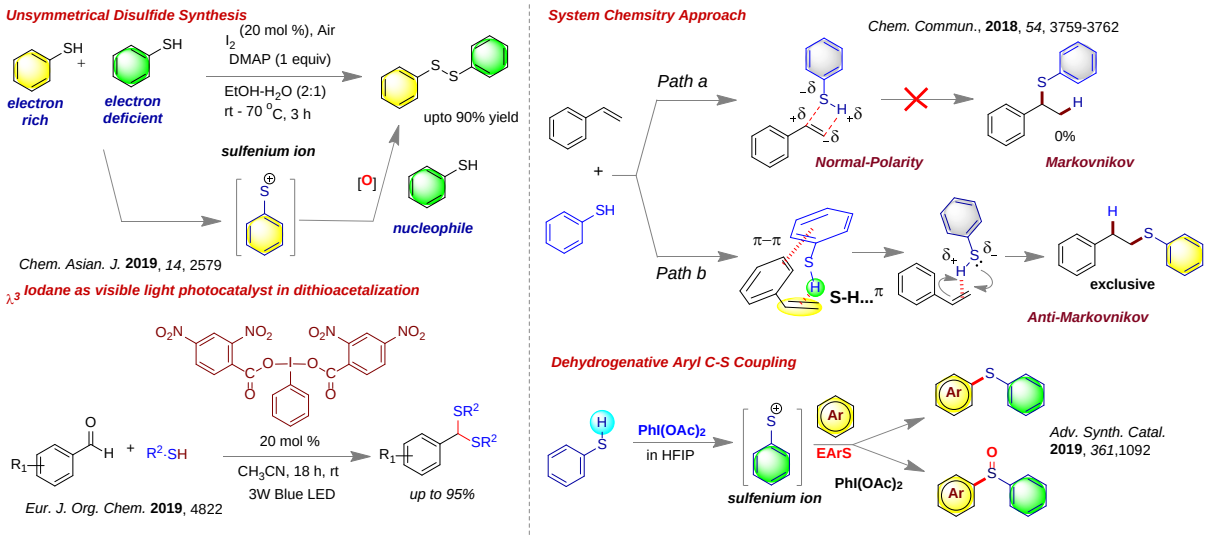

Figure 1

References and Notes:

(1) Bose, A.; Maiti, S.; Mal, P. In *Noncovalent Interactions in Catalysis*; Mahmudov, K. T., Kopylovich, M. N., Guedes da Silva, M. F. C., Pombeiro, A. J. L., Eds.; The Royal Society of Chemistry: 2019, p 188.
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(5) Choudhuri, K.; Mandal, A.; Mal, P. *Chem. Commun.* **2018**, *54*, 3759.

Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

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Host: Dr. Jonathan R. Nitschke, University of Cambridge, UK

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Mechanistically guided synthesis of phosphine-phosphite and implications in asymmetric hydrogenation

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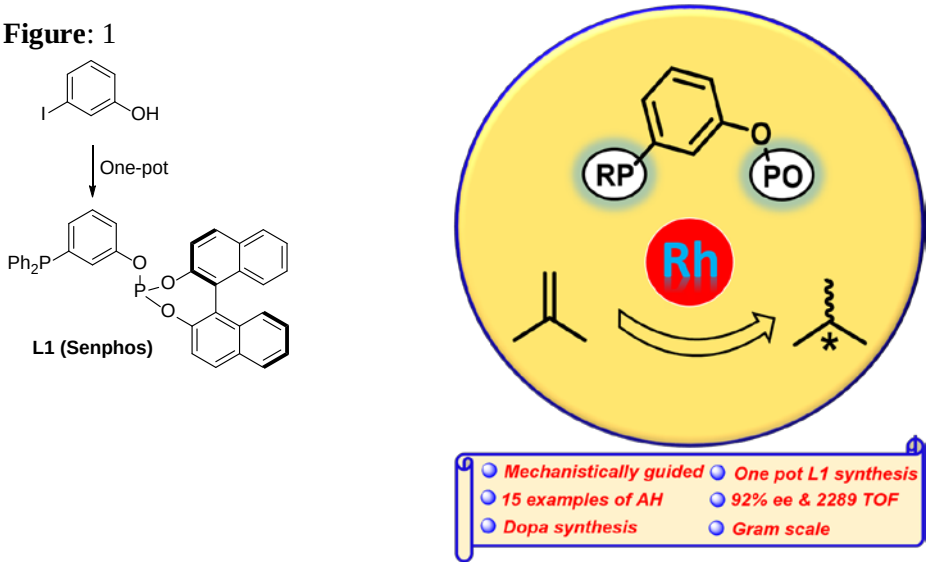
Abstract:

Synthesis of hybrid bidentate ligands such as BINAPHOS is a multistep and time consuming affair. Therefore, a paradigm shift can be achieved if hybrid bidentate ligands can be prepared in one step. However, there is hardly any report on the one pot, atom economic synthesis of a hybrid phosphine-phosphite. I shall present our efforts in this direction in general. In particular, one pot synthesis of hybrid ligand 4-(3-(diphenyphosphinaneyl)phenoxy)dinaphtho[2,1-*d*:1',2'-*f*][1,3,2]dioxaphosphepine (**L1**) will be presented.[1] After understanding the reactivity difference between an oxygen derived nucleophilic center versus a carbon based nucleophile using ^{31}P NMR spectroscopy, one pot synthesis of a hybrid ligand, Senphos (**L1**), has been achieved in very good yields (72%). Senphos, in the presence of rhodium catalyzes the AH of Methyl-2-acetamido-3-phenylacrylate and discloses an unprecedented turn over frequency (TOF) of 2289, the highest known for any phosphine-phosphite ligand, along with excellent enantio-selectivity (up to 88%). Thus, asymmetric hydrogenation of 15 different alkenes was successfully catalyzed by Senphos-Rh complex and high activity and enantio-selectivity (92%) has been achieved. The reaction operates under mild conditions of 1-2 bar hydrogen pressure, at room temperature, within 5-25 minutes.

Figure: 1



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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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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, 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. Currently he leads a team of highly motivated researchers in organometallics, (functional) polyolefins and renewable/degradable polymers. His scientific interests are- functional olefin polymerization, renewables to polymers, P-stereogenic supramolecular phosphines and asymmetric hydrogenation/hydroformylation. His honours and awards include, fellowship from 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 2017-2018 by NCL-RF and Young Associate of Maharashtra Academy of Sciences. His work has led to 50 odd publications in international peer reviewed journals and he is an inventor on 12 patents.

New Strategies for the Synthesis of Complex Natural Products

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Abstract:
Our laboratory is interested in the synthesis of complex natural products. We select natural product targets for two reasons. First, some natural products possess valuable properties (such as biological activity in the context of human disease). If these chemicals cannot be obtained easily in large amounts from their natural sources, the laboratory synthesis of natural products provides a unique opportunity to study their activity in more detail for the purpose of benefiting human society. Moreover, the potential to generate unnatural derivatives of these naturally occurring chemicals with more potent or unique biological activities can be realized most effectively through chemical synthesis. Secondly, natural products provide an opportunity for learning new lessons in chemical reactivity and synthetic strategy, which drives the field of chemical synthesis forward. A common feature of all of our total synthesis projects is the central role of metal catalysis. We will describe the assembly of the complex molecular architectures of various natural products.

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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

Dr. Uttam K. Tambar
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Twitter: @TambarLab

Dr. Uttam K. Tambar moved from India to the United States in 1982. He received his A.B. degree from Harvard University in 2000 and his Ph.D. from the California Institute of Technology in 2006 with Professor Brian Stoltz. After he completed his NIH Postdoctoral Fellowship at Columbia University with Professor James Leighton in 2009, he began his independent research career at UT Southwestern Medical Center in Dallas. He is currently an Associate Professor in the Biochemistry Department and a W. W. Caruth, Jr. Scholar in Biomedical Research. The Tambar lab is interested in asymmetric catalysis, natural product synthesis, and medicinal chemistry. Dr. Tambar has authored >40 publications, and he is the inventor on two cancer-related patents. He has delivered >100 invited lectures around the world. Dr. Tambar has been a consultant for pharmaceutical companies, including Peloton Therapeutics. Dr. Tambar has been recognized by several awards, including the Welch Foundation Norman Hackerman Award, Alfred P. Sloan Foundation Research Fellowship, NSF Faculty Early Career Development Award, and Thieme Chemistry Journal Award. He is currently Chair of the Organic Chemistry Graduate Program at UT Southwestern Medical Center, and he is Co-Leader of the Chemistry & Cancer Program at the Simmons Comprehensive Cancer Center.

Alkoxyamide as A Phase Transfer Catalyst for Bromocyclization, and Bromination of (*Hetero*)Aromatics in Lipophilic Solvent

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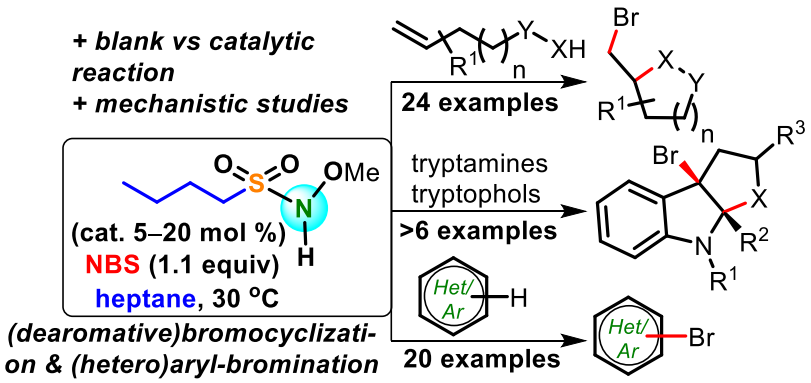
Abstract:

The use of electrophilic bromine for bromocyclization and related transformations to achieve promising brominated compounds has inspired the discovery and development of new brominating agents along with the catalyst that activates the brominating agents as well as the substrate.[a] In this line, a successful method requires sufficient and controlled amount of electrophilic bromine and good solubility of the reagent and the catalyst in the reaction solvent. However, a solid-liquid phase transfer approach is important to carry out a more practical bromo-functionalization when a lipophilic solvent is used alongwith an *N*-bromoamide reagent.[b]

The famous alpha-effect of the lone pair of electrons present in methoxylamine has been exploited as the guiding principle of the catalyst design in this work.[c] The alkoxamide such as *N*-alkoxy-sulfonamide facilitates acceptance as well as the delivery of bromonium species from N-bromosuccinimide to the unactivated alkenes or (*hetero*)aromatic ring via *N*-bromosulfonamide formation resulting in an effective alkoxamide-catalysis which can be further tuned to phase-tranfer catalysis. Thus, bromocyclization and bromination of (*hetero*)aromatics have been reported with broad substrate scope in addition to the comparison with the corresponding uncatalyzed reaction. Basic NMR-experiments have also been performed to understand the kinetics and the mechanism of the catalysis.



Scheme. Alkoxyamide: Phase Transfer Catalyst for Bromocyclization, and Bromination of (*Hetero*)Aromatics in Lipophilic Solvent

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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Dr. Modhu Sudan Maji born in 1982 and did his schooling from his native place Howrah, WB. He completed BSc in Chemistry (honors) from University of Calcutta in 2003, and stood second in the University. During his MS from IISc, Bangalore, he worked on ´´An Exploratory Approach Towards the Bioactive Marine Natural Product Tetrodotoxin`` with *Prof. Goverdhan Mehta*. In 2009, he completed his PhD under the guidance of *Prof. Armido Studer* from University of Muenster, Germany. Following this he received prestigious Alexander von Humboldt Fellowship and completed 3.2 years of post-doctoral research with *Prof. Magnus Rueping* of RWTH Aachen University, Germany. After another short post-doctoral research stay with *Prof. Martin Oestreich* of Technical University Berlin, Germany, he joined the Department of Chemistry of IIT Kharagpur as assistant professor in December 2013; where he is currently working as associate professor. His major research topics are asymmetric-organo-catalysis, multi-catalysis, C-H-bond functionalization, new catalyst development and natural product total synthesis. He has published 29 research papers in renowned journals.

Awards / Honors / Membership:

- Alexander von Humboldt Fellowship, Germany. (2010-2012)
- First Class Second in B.Sc. (Chemistry Honours) in the University of Calcutta, Kolkata, India. (2003)
- D. K. Mitra Gold Medal awards for securing the highest mark in Chemistry Department of Ramakrishna Mission Residential College, Narendrapur, Kolkata, India. (2003)
- INSPIRE Faculty Award from the DST, New Delhi, India. (2014-2019)
- Life member of Chemical Research Society of India.

Total Synthesis of Alkaloids of Biological Relevance

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& Department of Chemistry, IISER Bhopal, Bhauri, Madhya Pradesh, India
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Abstract:
Nature produces a variety of complex natural products and majority of these are isolated in entioenriched form (Figure). As these are isolated from Nature in limited quantity (mostly in mg scale), total synthesis endeavours can play a crucial role in bioactivity evaluation by providing access in significant quantity.[1-2]

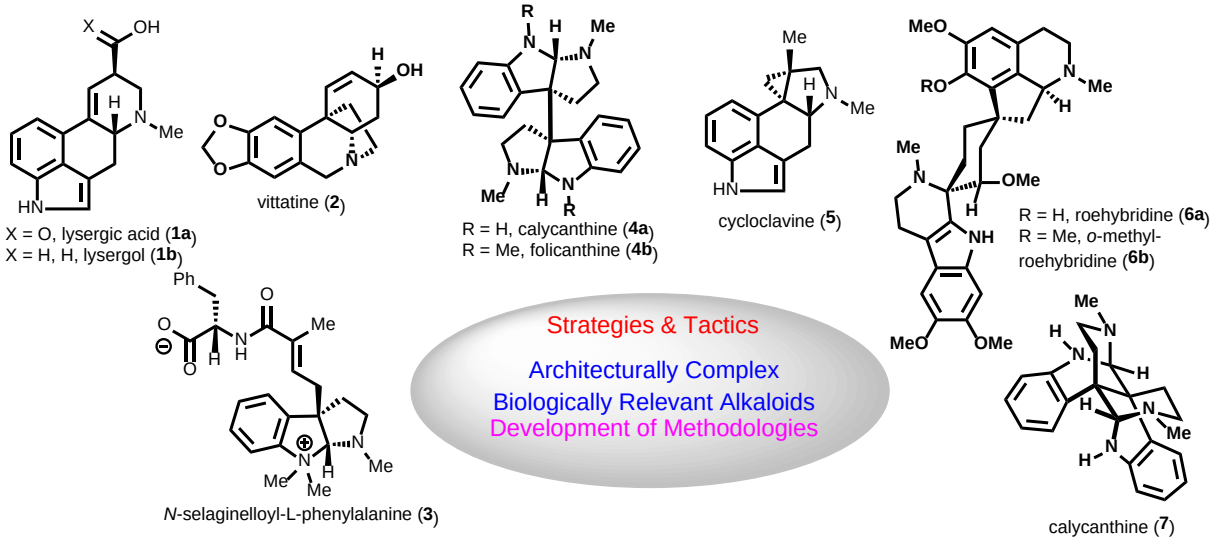

Figure. Naturally occurring architecturally complex alkaloids.

Towards this, catalytic asymmetric construction of organic molecules sharing all-carbon quaternary stereocenter is one of the challenging aspects of synthetic organic chemistry.[3] Towards this direction, naturally occurring alkaloids (Figure 1) with impressive diversity of biological activities drew our interest.[4] Our synthetic endeavors towards the total syntheses of these architecturally complex alkaloids via catalytic asymmetric methods will be discussed.[5]

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Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Group Homepage: https://home.iiserb.ac.in/~alakesh/index.html

Education:
2000 M. Sc. Banaras Hindu University
2006 Ph. D. IIT Kanpur, India (Synthetic Organic Chemistry) (Supervisor: Prof. Vinod K. Singh); 2006-2009 Postdoc with Prof. Richmond Sarpong, University of California at Berkeley; California, USA
December, 2009- November, 2013 Assistant Professor, IISER Bhopal
November, 2013- January, 2018 Associate Professor, IISER Bhopal
January, 2018-till date Professor, IISER Bhopal
May, 2019-till date Professor, IISER Kolkata

Awards & Honours:
Young Scientist Award by CRSI, India (July, 2018);
Young Scientist Award by the BRNS, DAE (2011-2014);
DST Fast-Track Project for Young Scientist (March, 2013-February, 2016);
GRC Award by Chair, 17th GRC on Stereochemistry (2008), RI, USA

After receiving M.Sc. degree in Organic Chemistry from BHU, Alakesh obtained his Ph.D. in synthetic Organic Chemistry under the supervision of Professor Vinod K. Singh from the Department of Chemistry, IIT Kanpur in Sept. 2006. Immediately afterward, he moved to the College of Chemistry, University of California at Berkeley, where he held postdoctoral position in the research group of Professor Richmond Sarpong. During his stay at Berkeley, he completed concise total synthesis of '*lycopodium alkaloids*' lyconadin A which received considerable attention from the synthetic community. During his Postdoctoral research, he received the GRC (*Gordon Research Conference*) award to Post-docs by Chair, 17th GRC on Stereochemistry (2008), RI. In Dec. 2009, he left Berkeley and joined IISER Bhopal, where he is currently a Professor. In May, 2019, he moved to IISER Kolkata (on long leave from IISER Bhopal) to set a research lab. on Natural Product synthesis.
The research focus of the AB research group includes the total synthesis of architecturally interesting biologically active natural products that provide an ideal platform for the invention of new strategies and highly selective organic transformations. Recently, his total synthesis of pyrroloindoline alkaloids had been highlighted in '*Organic Chemistry Portal*' as '*The Bisai Synthesis of (-)-Physovenine*'. He is the recipient of *Young Scientist Award* by the CRSI, INDIA (2018); and BRNS, DAE (2011) through research grant. Apart from academics, he has served IISER Bhopal in different administrative capacities such as Conveners, *DUGC and DPGC* of Department of Chemistry; Member, *Departmental Faculty Advisory Committee* (DFAC-Chemistry); Coordinator, *Outreach Activities*, Chairperson, *Health Center User Committee* (HCUC); *Dean of the Faculty Affairs* (DoFA) and *Chief Vigilance Officer* (CVO). He has also served as *Dean of the Faculty Affairs* (DoFA) for IISER Berhampur for initial period (*Mentor Institute*: IISER Bhopal).

A Nickel Catalysed Alcohol Oxidation and *N*-alkylations Mediated by Hydrogen Atom Transfer

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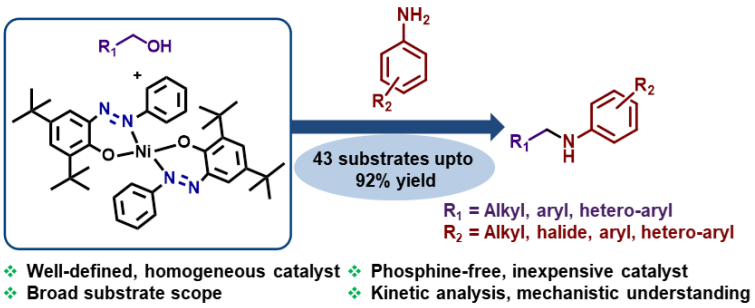
Abstract:
The N-alkylation of primary amines to higher amines is of importance for the synthesis of various biologically active molecules. Previous reports for the synthesis of secondary and tertiary amines via alkylation of primary amines involve toxic chemicals and harsh reaction conditions. In the present work, we attempt to explore environmentally benign synthesis of higher amines employing inexpensive and readily available alcohols as alkylating agents, generating water as the only byproduct. The redox non-innocent ligand backbone in the catalyst plays an important role to do efficient conversion. Indeed, it has been observed that a hydrogen atom transfer (HAT) is the crucial step to further alcohol oxidation, which is in stark contrast to traditional M-L bifunctional activation of a bond.[1] Detailed kinetic studies and isotope effects elucidate the mechanistic sketch further which helps us to extend the scope of the reaction in broader field.

Figure:



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Bains, A.K.; Kundu, A.; Yadav, S.; Adhikari, D. *ACS Catal.*, **2019**, 9, 9051-59

Flash Talk & Poster Presentation

International Conference on Organometallics and Catalysis (ICOC 2020)

Bio-Sketch of Speaker

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Debashis completed his Masters from IIT Kanpur and Ph.D. from Indiana University, Bloomington followed by a postdoctoral stint in Northwestern University. Before coming back to India he taught in Indiana University as a lecturer. He started his indepemdemt carrier in 2016 as an Assistant professor in IISER Mohali. His group is mainly focussed on utilizing redox active backbones for base metal catalysis and performing small molecule activation. The group strives to understand the detailed electronic structure of molecules both via spectroscopic methods and computational means with an aim of further designing the catalyst.

POSTER PRESENTATION

Bottleable Neutral Carbon Centered Radical for Single Electron Transfer Catalysis

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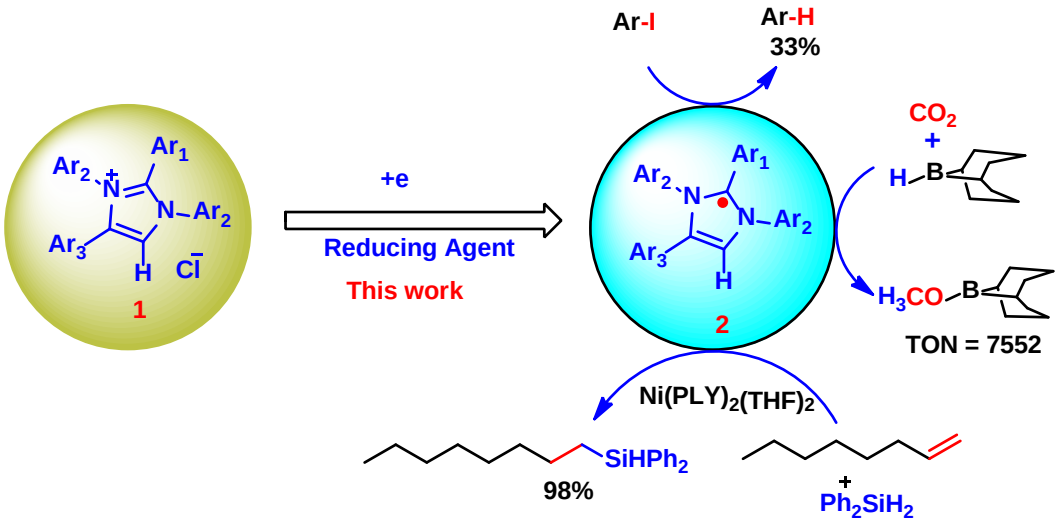
Abstract:
It's been nearly 120 years since the first stable carbon centered neutral radical was reported but only a limited no of radicals are characterized by their solid state structure till date due to low stability.[1-2] In this regard, substituted imidazolium salts may be a good precursor for synthesizing stable neutral carbon-centered radicals.[3-5] One electron reduction of imidazolium salt (**1**) resulted in the formation of imidazolium radical (**2**). The solid state characterisation of imidazolium radical (**2**) was accomplished by single crystal X-ray crystallographic study. Spin density calculation shows that major electron density lies on the C-2 carbon atom. In this poster, we report the synthesis of a carbon centered imidazolium based neutral radical (**2**) and its application as an electron transfer agent in a number of catalytic organic transformations such as in activation of aryl-halide bond, in alkene hydrosilylation and in catalytic reduction of CO_2 to methoxyborane; all under ambient conditions.

Figure:



➢ A. Das, S. K. Mandal, Unpublished work.

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Development of Template Assisted Distal *para*-C–H Functionalizations

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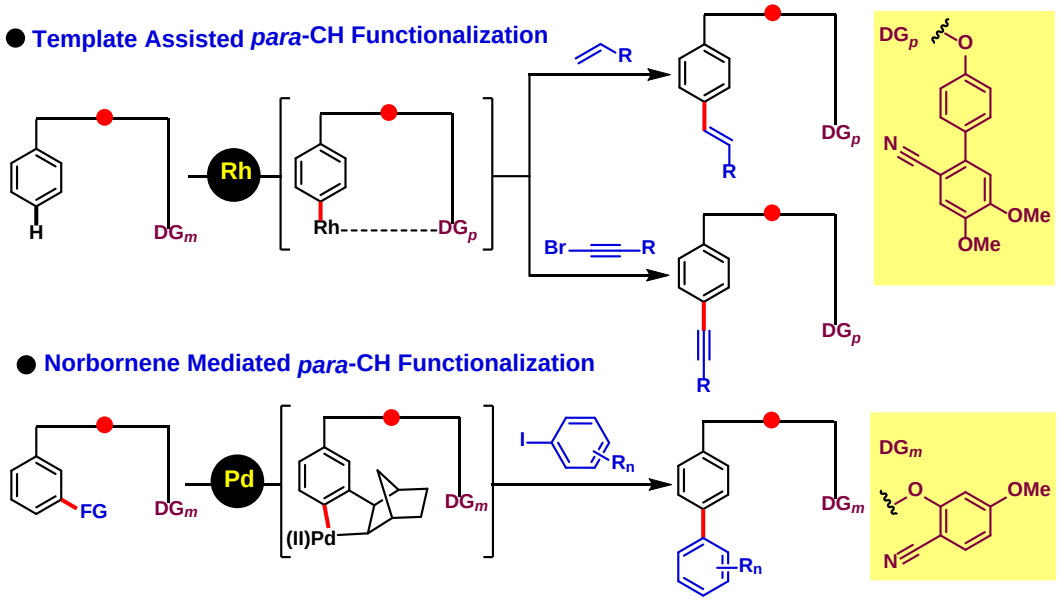
The emergence of functionalization and site-selectivity are the key factors in synthesizing privilege class of complex molecules. Distinguishing the subtle reactivity differences and the innate inertness of multiple C–H bonds present in an arene set-up posed the major challenge in the realm of site selective C–H functionalization of arene cores. Last few decades have witnessed a rapid insurgence of regioselective C–H functionalization *via* directing group (DG) assistance to remoulded the process of functional group installation. In its itinerary thus far, *ortho*- and to some extent *meta*-C–H functionalizations have been explored. While the scope of *meta*-C–H functionalizations is broadening, the similar success story remained elusive till 2015, owing to the necessity for formidable formation of 15-17 membered macrocyclic metallacycle. Nonetheless, our group has developed easily recyclable, novel Si-containing biphenyl-cyano based D-shaped assembly to ensure *para*-selective C–H functionalization under palladium catalysis.[1] However, in search of alternative transition metals, herein we disclosed the rhodium catalysed distal *para*-C–H alkenylation[2] and alkynylation protocol. Rhodium catalysis is advantageous in many ways; such as use of cheaper oxidant, inexpensive solvent and certainly a new ligand system that might be helpful in manipulating the stereo synthetic outcome. A complementary path to achieve distal *para*-C–H functionalization has also been achieved where 2-hydroxy-4-methoxybenzonitrile is used as *meta*-DG and in presence of norbornene derivative as a transient mediator to produce selective *para*-arylated arenes.



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NHC-Catalyzed [3+3] Annulation of Thioamides and Modified Enals for the Enantioselective Synthesis of Functionalized Thiazinones

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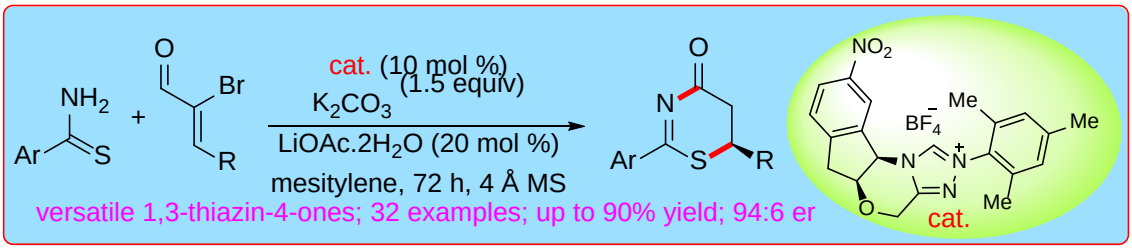
Organocatalysis using N-heterocyclic carbenes (NHCs) are widely used for the construction of heterocycles, carbocycles and acyclic molecules, where carbenes are responsible for the umpolung of the electrophile involved in the transformation.[1] NHCs are also useful for catalyzing non-umpolung transformations, and one of the important mode of reaction in this domain is via the generation of α,β-unsaturated acylazolium intermediates.[2,3] Herein, we present NHC-catalyzed [3+3] annulation of thioamides[4] with modified enals allowing the enantioselective synthesis of functionalized 1,3-thiazin-4-ones is reported. The NHC generated from the chiral triazolium salt was optimal and the reaction is initiated by the thia-Michael addition to catalytically generated α,β-unsaturated acylazolium intermediates derived from 2-bromoenals followed by intramolecular cyclization. This operationally simple procedure offers a straightforward and rapid access to target compounds in moderate to good yields and er values.[5,6]



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2. For reviews on α,β-unsaturated acylazoliums, see: (a) Mondal, S.; Yetra, S. R.; Mukherjee, S.; Biju, A. T. *Acc. Chem. Res*. **2019**, *52*, 425. (b) Zhang, C.; Hooper, J. F.; Lupton, D. W. ACS Catal. 2017, 7, 2583.
3. For selected reports from our group, see: (a) Mondal, S.; Ghosh, A.; Mukherjee, S.; Biju, A. T. *Org. Lett.* **2018**, *20*, 4499. (b) Mukherjee, S.; Ghosh, A.; Marelli, U. K.; Biju, A. T. *Org. Lett.* **2018**, *20*, 2952. (c) Yetra, S. R.; Mondal, S.; Mukherjee, S.; Gonnade, R. G.; Biju, A. T. *Angew. Chem., Int. Ed*. **2016**, *55*, 268.
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6. For a closely related independent contribution, see: Changyi, L.; Wu, S.; Xu, J.; Chen, L.; Zheng, P.; Chi, Y. R. *Org. Lett.* **2019**, *21*, 9493.

Catalytic Asymmetric Sequential Allylations of Dimeric 2-Oxindoles

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Alkaloids sharing all-carbon quaternary stereocenter is one of the challenging aspects of synthetic organic chemistry when it comes in asymmetric construction. The situation becomes more difficult when the target molecule contains contiguous all-carbon quaternary stereocenters. Towards this, naturally occurring cyclotryptamine alkaloids and related bis-indole alkaloids (**1-4** in Figure 1) with impressive diversity of biological activities drew our synthetic interest.[1] Because of extreme steric congestion about the C3a-C3a' σ-bond and the attendant labiality of this linkage (in **1a-b**), the total syntheses of these alkaloids possess synthetic challenge to the synthetic community.

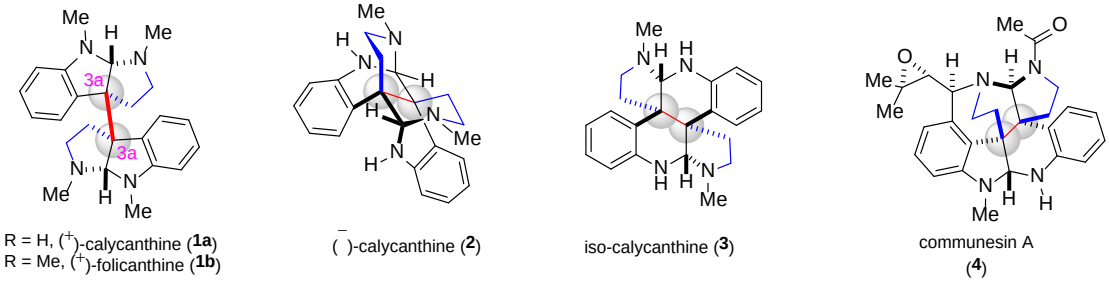
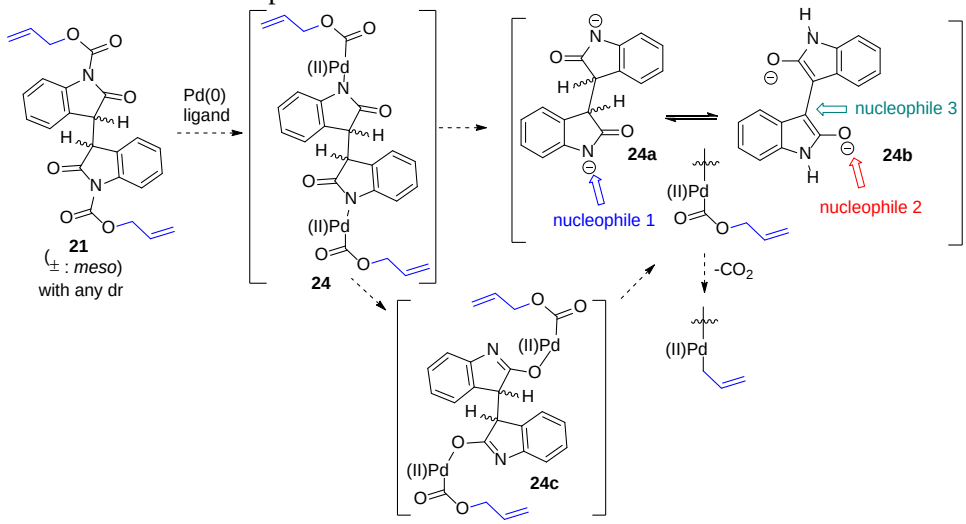


Figure 1: Selected cyclotryptamine alkaloids (**1-4**).

So far as biological activities are concerned, congeners of this family are reported to be potent competitive substance P antagonist with respect to human neurokinin-1 and the cholecystokinin B receptor.[1] For a unified strategy of these targets,[2] we explored novel methodologies that addresses installation of all-carbon quaternary stereocenters (Scheme 1).[2] Our synthetic endeavors using a Pd(0)-catalyzed chemoselective allylations and its application in total synthesis of dimeric hexahydropyrrolo-[2,3*b*]-indoline alkaloids will be presented.[3]



Scheme 1. Our proposed DYKAT for asymmetric total synthesis of folicanthine (**1b**).

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Catalytic Platform for Hauser Annulations

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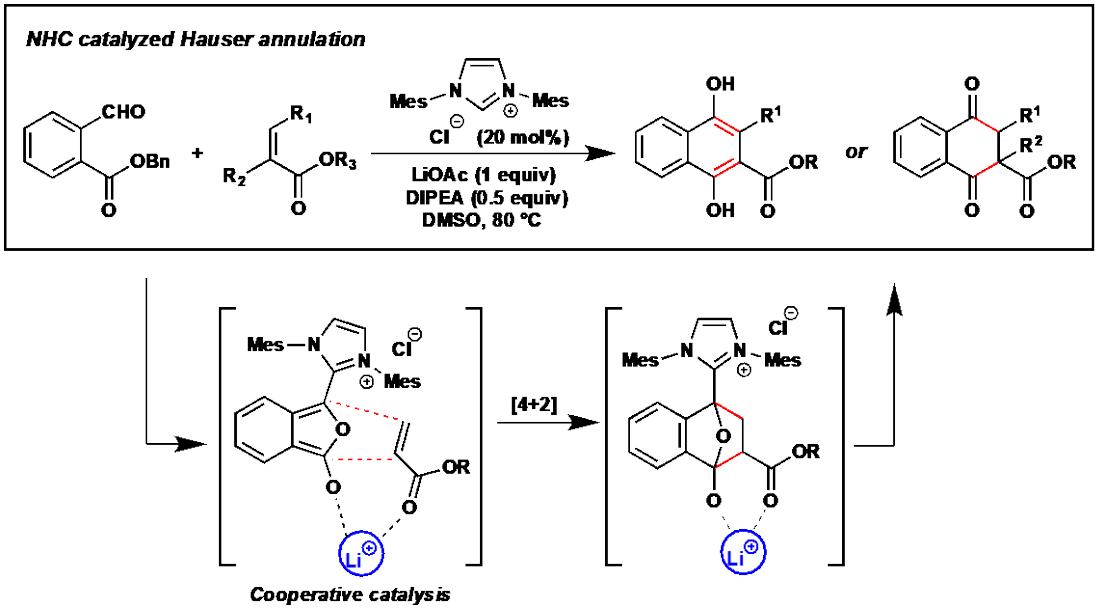
Abstract:
The traditional Hauser annulation is a great synthetic tool for installment of benzannulated scaffolds in natural products. Despite its versatility to synthesize complex benzannulated products, the synthesis of the substituted phthalides as starting materials in the traditional Hauser annulation can be difficult and requires toxic reagents.[1] We have developed the first catalytic Hauser annulation by employing NHC-mediated umpolung chemistry from readily accessible, step-economic, and non-toxic starting materials. The reaction proceeds under mild reaction conditions and is compatible with various functional groups. The application of our methodology to produce medicinally valuable products and natural products is currently under investigation.[2]



Highlights of our catalytic Hauser annulation methodology

- Use of non-toxic and readily accessible starting materials contrary to traditional Hauser annulations
- Mild reaction conditions and high functional groups tolerance
- 25 examples (35-85% yield)
- Cooperative catalysis and [4+2] cycloaddition

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Mechanistic Investigation of Dinitrogen Reduction at the Titanium Center

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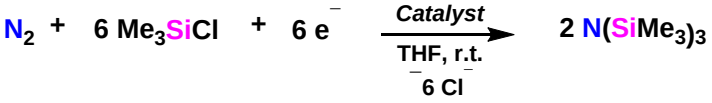
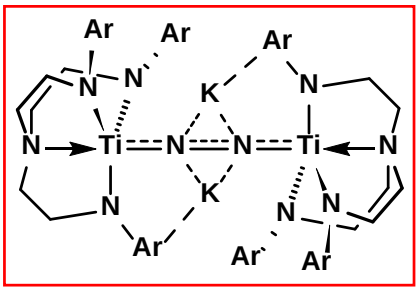
Abstract:

Fixation of atmospheric dinitrogen into some value-added products under ambient conditions is an uphill task owing to the inertness of the N_2 molecule with its extremely strong N≡N bond (BDE = 944 kJ mol^{-1}), zero dipole moment and large HOMO-LUMO gap.[1] To overcome this challenge, normally highly reduced transition metal complexes are employed to provide electrons to activate N≡N bond for further functionalization.[2] So far catalytic functionalization of dinitrogen was primarily achieved using mid-transition metals such as Cr, Mo, Fe, or Co.[3] In contrast, complexes based on early-transition metals that can catalyze nitrogen fixation are still very scarce.[4] Taking advantage of the 3,5-dimethylphenyl substituted triamino-amine ligand H_3(Xy-N_3N) (Xy-N_3N = {(3,5-$Me_2C_6H_3$)NCH_2CH_2}$_3$N^{3-}), herein we present a series of titanium complexes, those catalyze the conversion of dinitrogen into N($SiMe_3$)$_3$ under ambient conditions with catalytic turnovers of up to 16.5 per titanium atom (Figure 1).[5] In addition, a detail mechanistic study of the catalytic cycle of dinitrogen reduction will be presented here.



Catalytic turnover up to 16.5 per titanium atom



Catalyst

***Figure 1*:** Catalytic fixation of N_2 to N($SiMe_3$)$_3$ at the titanium center; Ar = 3,5-$Me_2C_6H_3$.

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Low-Valent Phosphorus Compounds in Catalytic Functionalization of Greenhouse Gas

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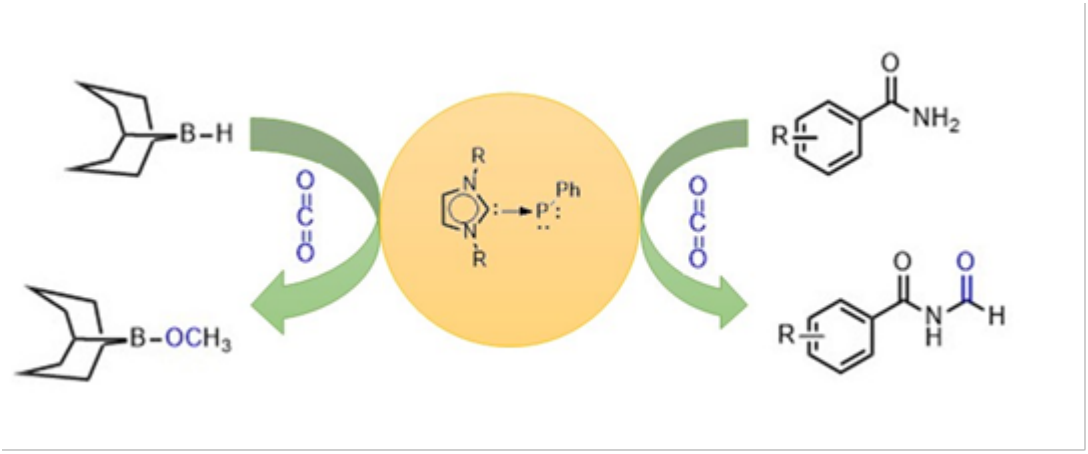
Abstract:
Phosphinidenes P-R represent the phosphorus analogues of carbenes (R-C:) consisting of monocoordinated phosphorus atom with two lone pairs of electrons and a vacant orbital.[1] Stabilization of singlet phosphinidene can be achieved by introducing an N-heterocyclic carbene unit to the phosphorus centre.[2] Despite the synthetic advancement, phosphinidenes were not reported for any catalytic application till date. The availability of two pairs of electrons can be judiciously tuned as nucleophile for various organic transformations by varying the substituents and carbene backbone. Herein we report use of phosphinidene as catalyst for simultaneous reduction and reductive functionalization of CO_2 into methanol and formylation of chemically inert primary amides (Figure. 1).

Figure:



➢ P. Sreejyothi, S. K. Mandal, Unpublished work

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Aromatic Doubly Reduced Odd Alternant Hydrocarbon for Catalytic Activation of Aryl Halides at Room Temperature

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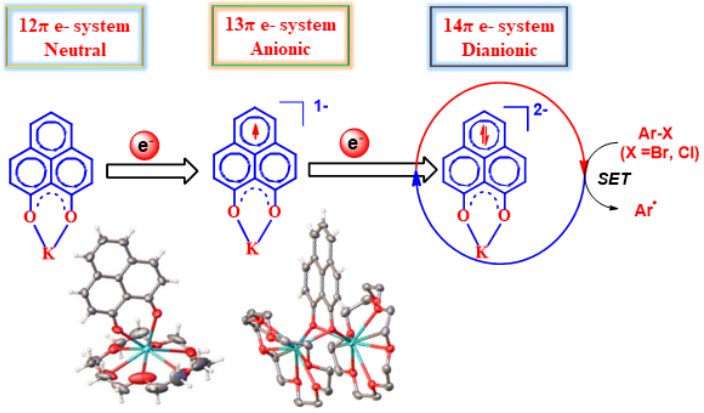
Abstract:
Aryl halides (mainly bromides and chlorides) are considered as the challenging substrate to activate in C-C cross-coupling reaction which is mostly accomplished by transition metal based catalysts. To avoid the use of transition metal in aryl halide activation several methodologies were introduced in last few years.[1-3] All these methodologies are stimulated by a constant external energy source such as heating, light or cathodic reduction. This work develops a new strategy of aryl halide activation towards direct C-H arylation by a new redox window between monoreduced and doubly reduced odd alternant hydrocarbon moiety.[4-6] For the first time, the radical anionic phenalenyl (PLY) moiety has been isolated in solid state in the form of monoreduced PLY-K complex. The double reduced species of PLY-K complex is also characterized. NICS values and AICD plots of three different redox states (neutral, anionic and dianionic) of PLY-K indicate that there is no significant aromaticity loss of phenalenyl moiety. This unique property of this PLY-K complex makes it a catalytically active super electron donor which can activate aryl halides at room temperature without using any external stimuli. A combined approach of experiment, theory and solid state characterization help to understand the insight of this catalytic process.

Figure:



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Efficient Transfer Hydrogenation of Ketones using MeOH as Liquid Organic Hydrogen Carrier

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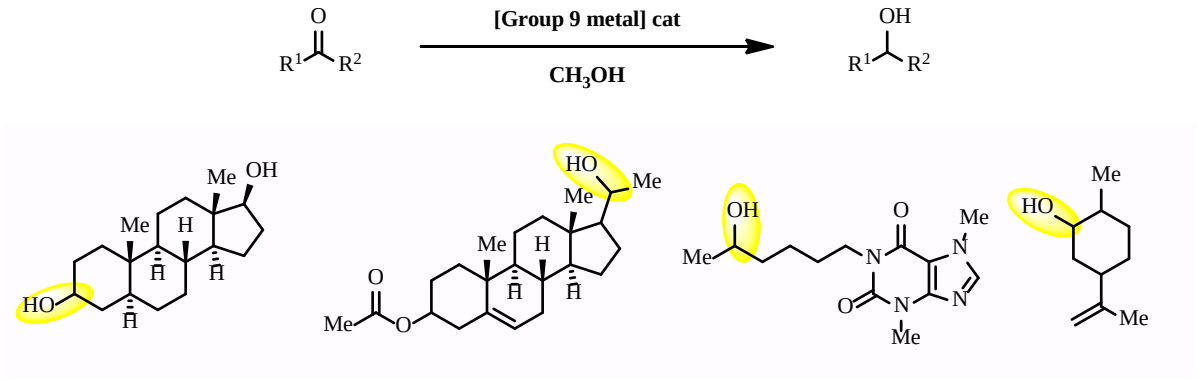
Abstract:

Reduction of carbonyl compounds is one of the most fundamental transformation practiced in both academia and chemical industry. Traditionally, stoichiometric amount of reducing agents or hazardous hydrogen gas with transition metals are employed for the reduction of ketones into their respective alcohols. However, transfer hydrogenation of ketones using catalytic amount of transition metals is a viable alternative for such transformations as they proceed via metal-hydride formation and avoid the release of free hydrogen gas. Though such concept is explored using isopropanol, HCOOH etc. as Liquid Organic Hydrogen Carrier (LOHC)[1] but so far, only a handful of reports are there where methanol act as a hydrogen source.[2] The prime reason behind this is that dehydrogenation of methanol is an uphill process (63.7 kJ/mol) and thus, challenging. So far, methanol-water reformation process demands high temperature (>200 °C).[3] In this regard, we herein present, an efficient and practical transfer hydrogenation of ketones by homogeneous group-9 metal/ligand system using methanol as LOHC under mild reaction conditions. The catalytic system works well under catalytic amount of base, do not require any stoichiometric reducing agents, additional organic solvent, special equipment or harsh conditions. The more detailed results and mechanistic investigations will be discussed.[4]



Scheme: Ir(III) Catalyzed Transfer Hydrogenation of Ketones using Methanol as Hydrogen Source.

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Lewis Acid-Catalyzed Ring-Opening 1,3-Aminothiolation of Donor-Acceptor Cyclopropanes Using Sulfenamides

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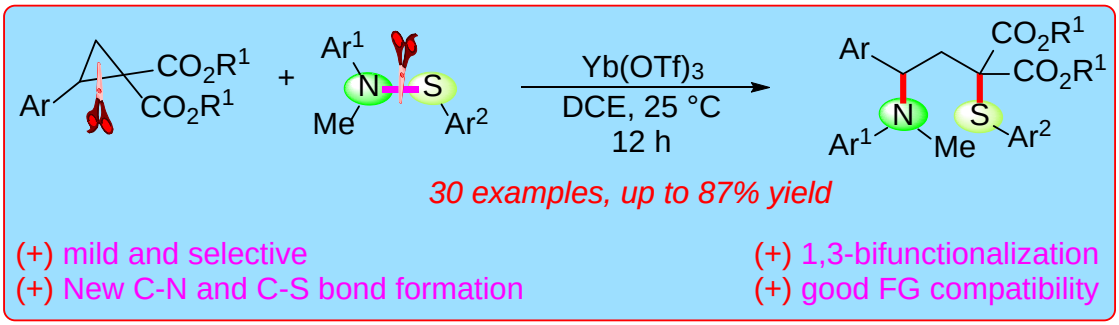
(avishekguin@iisc.ac.in)

Abstract:

Donor-acceptor (D-A) cyclopropanes are one of the versatile polarized three-atom building blocks in organic synthesis.[1] In the recent years, 1,3-bifunctionalization of donor-acceptor cyclopropanes has been gaining more attention.[2] Herein, we demonstrate the $Yb(OTf)_3$ catalyzed mild and regioselective ring-opening 1,3-aminothiolation of donor-acceptor cyclopropanes using sulfenamides.[3] The insertion of the C-C σ-bond of D-A cyclopropanes into the S-N σ-bond of sulfenamides allows the synthesis of diverse γ-aminated α-thiolated malonic diesters in moderate to good yields (up to 87%) with good functional group compatibility. The stereospecificity of the reaction was demonstrated using enantiopure D-A cyclopropane and the preliminary study on the mechanism of the reaction has been provided.



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Poster Presentation (PP-11)
International Conference on Organometallics and Catalysis (ICOC 2020)

N-Heterocyclic Carbene Catalysed Desymmetrization of Cyclic-1,3-Diketones via α,β-Unsaturated Acylazolium Intermediates

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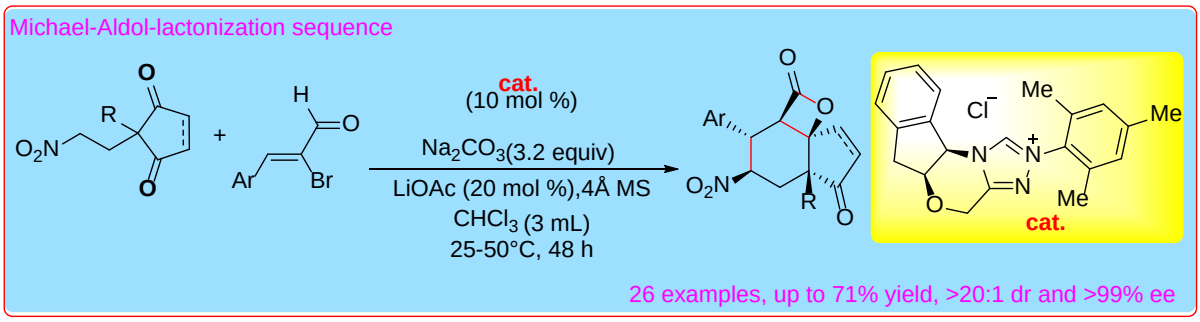
Desymmetrization is a powerful synthetic strategy for the construction of enantiomerically enriched complex molecules from simple achiral or meso starting material.[1] N-Heterocyclic carbenes (NHCs) have found application as versatile organocatalysts in a broad range of enantioselective transformations.[2] So the combination of desymmetrization and NHC catalysis has drawn global research interest in the field of asymmetric catalysis.[3] Herein, we present a desymmetrization strategy of cyclic-1,3-diketones for the enantioselective synthesis of tricyclic β-lactones with five contiguous stereocentres including two quaternary stereocentres. The NHC catalysed reaction of 2-bromoenals with cyclopentane-1,3-diketone derivatives proceeding via chiral α,β-unsaturated acylazolium intermediate allows the formation of the tricyclic β-lactones. The cascade reaction follows a Michael-aldol-lactonization sequence to afford the β-lactones in moderate to good yields with excellent enantioselectivity and diastereoselectivity.[4]



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N-Heterocyclic Carbene-Catalyzed Formal [6+2] Annulation Reaction via Cross-Conjugated Aza-Trienolate Intermediates

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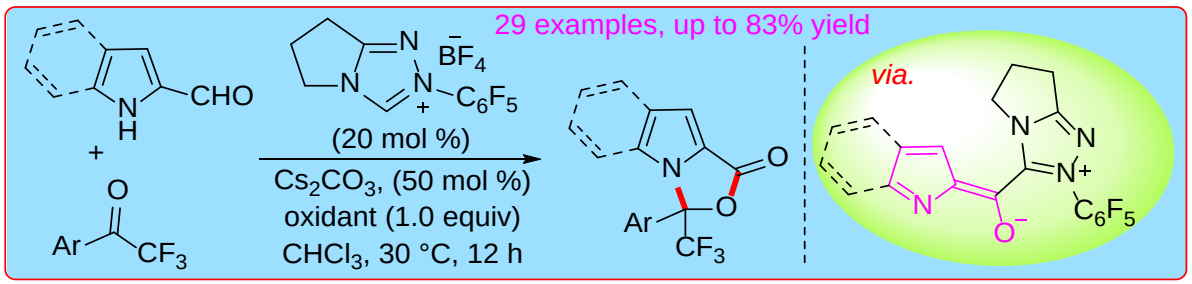
The diverse reactivity of N-heterocyclic carbenes (NHCs) in organocatalysis is due to the possibility of different modes of action.[1] Although NHC-bound enolates[2] and dienolates[3] are known, the related NHC-bound cross-conjugated aza-trienolates remain elusive. Herein, we demonstrate the NHC-catalyzed formal [6+2] annulation of nitrogen-containing heterocyclic aldehydes with α,α,α-trifluoroacetophenones leading to the formation of versatile pyrrolooxazolones.[4,5] The catalytically generated cross-conjugated aza-trienolates (aza-fulvene type) underwent smooth [6+2] annulation with electrophilic ketones to afford the product in moderate to good yields under mild conditions. Preliminary studies on the enantioselective version of the reaction as well as the DFT studies on mechanism are also provided.



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Mechanochemical C-H Bond Activation of Heterocycles: To Explore the Scope for 1st Row Transitional Metals

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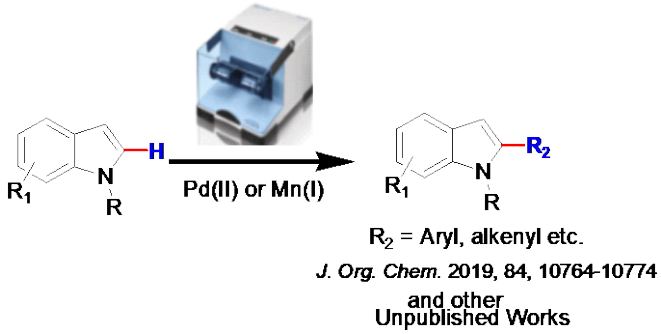
Abstract:

The development of efficient and environmentally friendly chemical processes for the preparation of biologically active and industrially useful molecules constitutes a major challenge for chemists in organic synthesis. A sustainable and "greener" method would focus on minimal to no use of solvents, reduction of other wastes, use of ambient conditions as well as shortening of reaction time, and developing more facile ways of product separation and purification. A mechanochemical process, which involves the input of mechanical energy for reactions such as ball-milling or grinding, facilitates most of the above mentioned features of sustainable methods and therefore, such strategies have emerged as attractive alternative to the traditional solution based synthetic methods [1]. Mechanochemistry has recently shown its prominence in the thriving area of C-H bond activation [2] but not many reports are available on utilizing 1st row transitional metals for the same [2b].

In this direction, we have recently started exploring the potential of mechanochemical agitation towards metal-catalyzed C-H bond activation of heterocycles (e.g. indoles) including 1st row transitional metal as catalysts (Scheme 1). The presentation will also cover our journey in the field of "mechanochemical organosynthesis" [3].



Scheme 1: Mechanochemical C2-selective C-H activation of indoles.

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Poster Presentation (PP-13)

International Conference on Organometallics and Catalysis (ICOC 2020)

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- **M. Sc.** from the University of Calcutta with specialization in Organic Chemistry in 1998.
- Postdoctoral stints: 1 year in Pusan National University, 2 years in POSTECH, South Korea.

Research and Teaching Experience:

Ten years of UG and PG teaching and Twelve years of Research (Post-PhD).
Total no. of Publications: 38 (all international); 2 patents; total citation: 1117; h-index: 18; i10-index 21.
International and National Conference Presentations/Talks: >25
ORCHID ID: orcid.org/0000-0002-6833-5531
Google Scholar: https://scholar.google.co.in/citations?user=fgxOj_MAAAAJ&hl=en

Research interests:

Mechanochemistry, Nanochemistry, Heterogeneous catalysis, Method development, Chemosensors etc.

Collaborations: University of Turin, Italy, BARC, Mumbai; NCL Pune, NIO Goa, Goa University, Sikkim University, Syngenta Bioscience Pvt. Ltd. Goa.

Membership of Professional Societies:

Member of Royal Society of Chemistry (MRSC); Member of American Chemical Society; Life member of Indian Association of Cultivation of Sciences; Life member of Chemical Research Society, India; Life member of Association of Carbohydrate Chemists and Technologists, India (ACCTI); Indian Society for Radiation and Photochemical Sciences (ISRAPS)

Projects: No. of projects completed: 06 (02 Gov. of India funded as PI (DST fast-track and CSIR); 02 industrial projects as PI; 02 Gov. of India funded as co-PI); Total budget of completed projects: approx. ₹. 8.4 million.

On-going projects: 1. DST-SERB project "A comprehensive study on mechanochemical sp^2 C-H bond activation in five-membered heteroaromatics in a Ball-Mill" (Project no. EMR/2016/002253), ₹.3.2 million, ongoing.

2. Design and synthesis of smart supramolecular dyes based on TPE modified PDI cucurbituril conjugates, BRNS, 3 years, ₹.2.8 million.

Selected Awards, Honours, Recognitions:

1. Recipient of BK 21 fellowship of Korea Government for Postdoctoral studies, 2006-2007.
2. CSIR travel grant for Singapore visit to attend ICMAT2017.

PhD students Supervised: 02 PhD (awarded), 01 RA, 04 ongoing PhD scholars, 02 master thesis, 18 project students.

High-Valent Cobalt-Catalyzed C-H Bond Functionalizations using Weakly Coordinating DG

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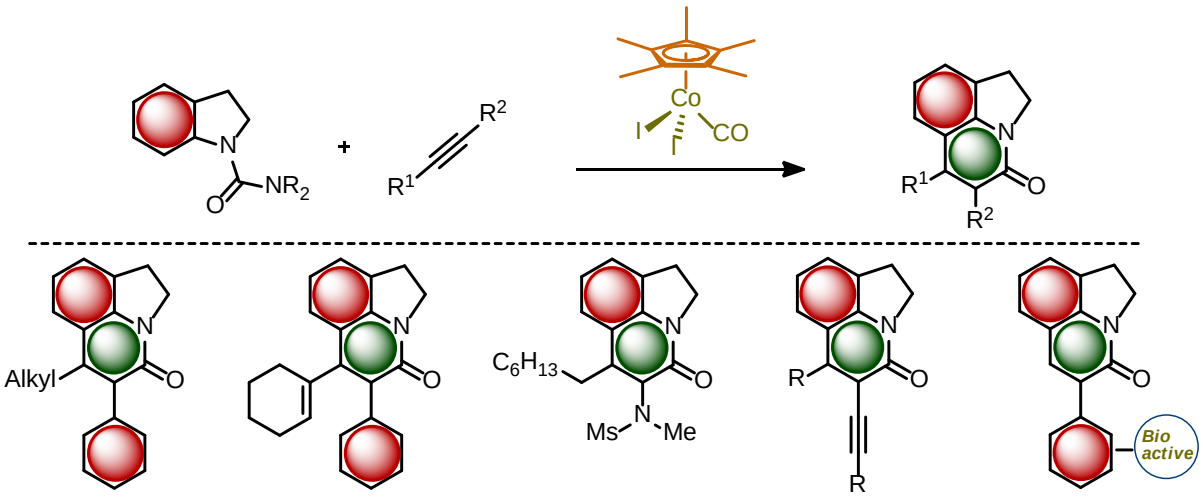
Abstract:
Transition metal catalyzed functionalizations of C-H bonds have gained great attention of chemist for formation of C-C, C-heteroatom bonds in a step- and atom-economical way. Various precious noble metals (e.g. Ru, Rh, Ir, Pd, Pt etc.) have been widely employed to serve the above mentioned purpose.[1] However, their low abundance and high cost limits their applicability and hence, enforces chemists to think for an alternative catalyst to carry out such transformations. Among the various 3d transition metal complexes, Cp*Co(III) complexes emerge as a promising alternative for such transformations. Strongly co-ordinating DGs such as pyridine, pyrimidine, imidazole etc. have been utilized for various C-H bond functionalizations however, the removal or modifications of such DGs require harsh conditions.[2] While the use of DGs such as carboxylic acid, carbonyl, amide or the DGs which gets utilized in the scaffold make the process much more synthetically viable.[3] The low Lewis acidity of 3d transition metals makes such processes more challenging as the coordinating atoms are also less Lewis basic thus, making the cyclometallated intermediates less stable. Herein, we have shown Cp*Co(III)-catalyzed annulations of *N*-carbamoyl indolines with various alkynes to provide biologically important indoline alkaloids in moderate to excellent yields along with high regioselectivity. To our delight, ynamide, *di*-yne and terminal alkynes have also afforded expected products in good-to-excellent yields (Scheme-1). Isolation of intermediates is currently ongoing in our laboratory to gain more insights about the reaction mechanism.



Scheme 1: Synthesis of various pyrroloquinolinone under Cp*Co(III)-catalysis.

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A Linchpin Approach to Access Drug–Pharmacophore Conjugate by Inverse Sonogashira at *meta*-Position

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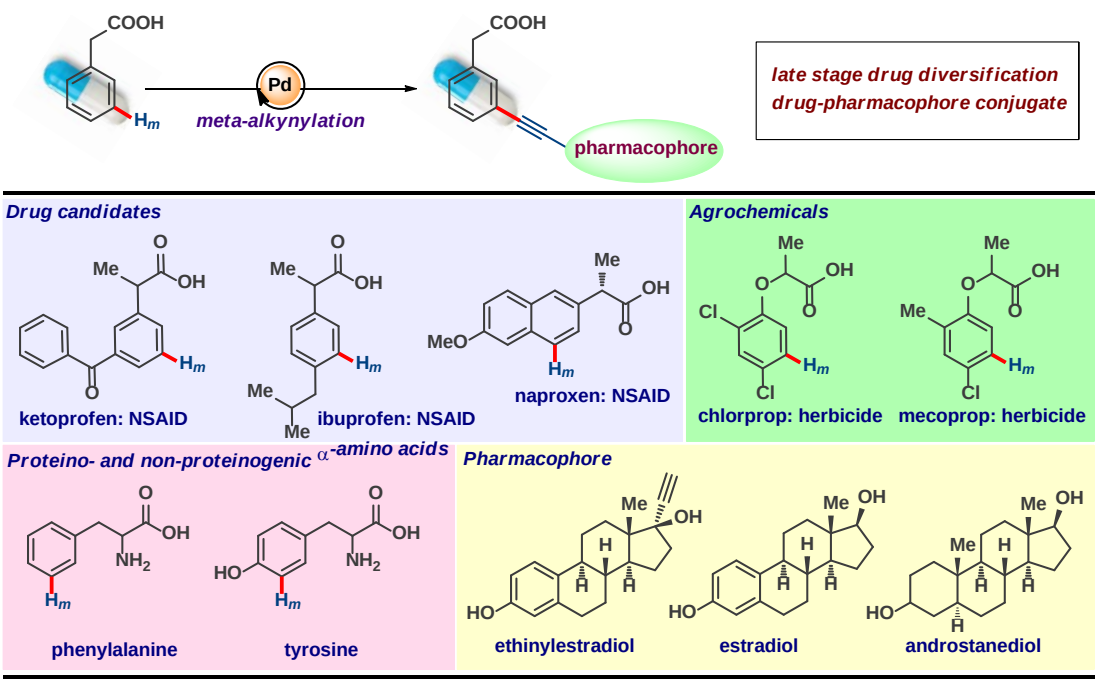
The late-stage functionalization (LSF) of pharmaceutical and agrochemical compounds by the site-selective activation of C–H bonds offers immediate access to diverse structural analogs and expands the accessible chemical space. We report a C–H functionalization LSF strategy that hinges on the use of an alkyne linchpin to assemble conjugates of sp^2-rich marketed pharmaceuticals and agrochemicals with sp^3-rich 3D-fragments and natural products. This is accomplished through a template-assisted inverse Sonogashira reaction that displays high levels of selectivity for the *meta*-position.[1] This protocol is also amenable to distal structural modifications of α-amino acids. The transformation of alkyne functionality to other functional groups further highlights the applicative potential. Computational and experimental mechanistic studies shed light on the detailed mechanism. Turnover-limiting 1,2-migratory insertion of the bromoalkyne coupling partner occurs after relatively fast C–H activation. While this insertion occurs unselectively, regioconvergence results from one of the adducts undergoing a 1,2-trialkylsilyl migration to form the alkynylated product. A heterobimetallic Pd–Ag TS, which is essential for product formation, is explicitly implicated in the β-bromide elimination step.



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Poster Presentation (PP-16)

International Conference on Organometallics and Catalysis (ICOC 2020)

Para-Selective Cyanation of Arenes by H-bonded template

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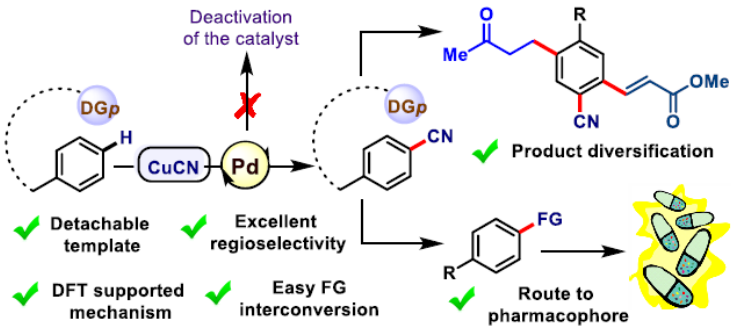
Cyanoarenes found in todays' advanced synthetic intermediates, various natural products and drug motifs. Presence of cyano/nitrile functional group can lead to various functionalities like carbonyl, carboxyl, amino or heterocyclic groups by synthetic modifications. Currently over 30 nitrile-containing pharmaceuticals are prescribed for a diverse variety of medicinal conditions with 20 in queue for clinical development. Also few drugs molecules like Etravirine (anti HIV agent), Periciazine (antipsychotic and neuroleptic), Vildagliptin (antidiabetic drug), Fadrozole monohydrochloride (nonsteroidal aromatase inhibitors for treatment of breast cancer), Tanaproget (nonsteroidal contraceptives), Etravirin, Dapivirin, Rilpivirin, Lersivirin (new class of anti-HIV drugs) and Citalopram (selective serotonin transport inhibitor) has cyano group. However, methods available to introduce cyano group relies on conventional way. So directed C□H cyanation will be offering more reliable solution to earlier methods which involves highly reactive diazonium intermediate. Present study includes template assisted *para*- selective cyanation of toluene derivatives, mechanical investigation and computational studies.



References:

Sandeep Pimparkar,[a,b,c‡] Trisha Bhattacharya,[a‡] Arun Maji,[a] Argha Saha,[a] Ramasamy Jayarajan,[a] Uttam Dutta,[a,b,c] Gang Lu,*[d] David W. Lupton*[b,c] and Debabrata Maiti*[a,b]
ChemRXIV, 2020, Preprint, **https://doi.org/10.26434/chemrxiv.11448690.v1**

Poster Presentation (PP-17)
International Conference on Organometallics and Catalysis (ICOC 2020)

Expanding Chemical Space by Late-Stage *Para*-Arylation of Drugs

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The late stage functionalization (LSF) is a technique in which C–H bonds are regarded as functional groups and points of potential diversification to generate new analogs of a lead structure without resorting to de novo synthesis. In the context of developing LSF technologies for drug diversification *via para*-functionalization, we became interested in the development of a directing group strategy for biaryl formation, conjugating a drug with an aryl group or the vice versa. The vast majority of drugs contain several polar functionalities, often as part of oxygen, nitrogen and sulfur heterocycles that are essential to maximize the drug–target interaction and maintain acceptable levels of pharmacokinetics and toxicity. These polar groups are often problematic in C–H activation as the presence of Lewis basic heteroatoms can promote catalyst poisoning or substrate decomposition. Overcoming these hurdles, herein, we report the palladium(II)-catalyzed highly *para*-selective arylation of arenes with aryl iodides as coupling partners to establish a broadly useful linchpin strategy for drug–aryl conjugation through this protocol. Through this coupling reaction, a wide range of pharmaceutically relevant drugs and natural products as the part of arene substrate or aryl iodides could be diversified selectively at *para*-position; thereby enhancing the chemical space for further studies.

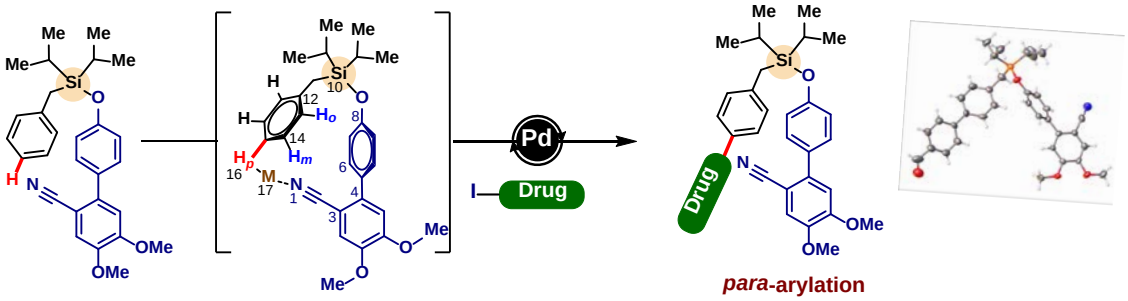

Figure 1. *Para*-C–H arylation of arenes.

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Orthogonal Selectivity in C–H Olefination: Synthesis of Branched Vinylarene with Unactivated Aliphatic Substitution

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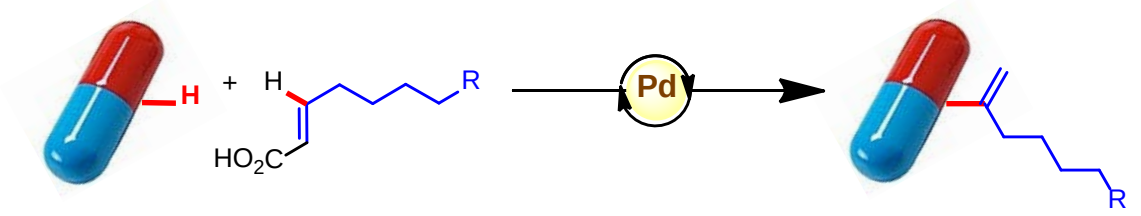
Oxidative coupling is a useful tool to synthesize vinylarenes. Despite remarkable successes in linear vinylarene, branched vinylarene synthesis has remained underdeveloped. Overcoming this limitation, herein we report a chelation assisted oxidative coupling to generate branched olefinated product in high yield. Exclusive branched selectivity was obtained using alkenyl carboxylic acid [1]. Detailed experimental studies combined with computational investigations suggest ß-migratory insertion, followed by a decarboxylation pathway is operative for the overall transformation. Direct functionalization of the unactivated C–H bond has emerged as a highly promising strategy for wide variety of chemical transformations. Unfortunately, the poor reactivity of the C–H bonds often restricts the scope of the transformation. The last two decades have witnessed milestone achievements in the direction of C–H activation using various transition metal catalysts. In this context, C–H olefination reaction has emerged as a major tool as it allows access to an array of pharmaceutical precursors, complex organic molecules, and drugs in a step and atom-economic way. Specifically, the palladium-catalyzed C–H olefination has become one of the attractive ways for accessing the olefinated products. In the current approach, we were able to utilize this reactivity by introducing a bidentate chelating ligand, which enables the regioselective olefination reaction with α,β-unsaturated carboxylic acids in a branched selective fashion. Further, we were able to olefinate a wide variety of pharmaceutical drugs and industrially relevant molecules, thus expanding our scope beyond the realm of simple organic molecules.



- Ibuprofen
- Naproxen
- Loxoprofen
- Flurbiprofen
- Homoveratric acid

- Directed C–H branched olefination
- Unactivated aliphatic substituent
- Excellent branched selectivity
- Hetero di-olefination

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N-Heterocyclic Carbene-Catalyzed Umpolung of Imines for the Enantioselective Synthesis of Dihydroquinoxalines

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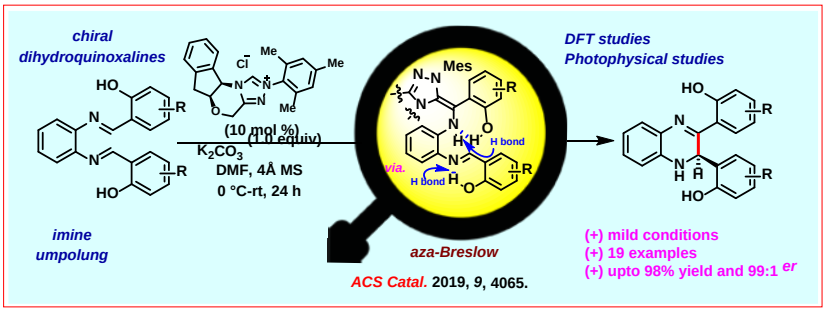
N-heterocyclic carbene (NHC) organocatalysis is widely employed for the umpolung of aldehydes[1], and recently to the umpolung of Michael acceptors[2] and aldimines.[3] Described herein is the NHC-organocatalyzed umpolung of aldimines for the enantioselective synthesis of nitrogen heterocycles. The bisimines generated from the condensation of 1,2-phenylene diamines and salicylaldehydes undergo intramolecular cyclization in the presence of a chiral NHC catalyst resulting in the formation of dihydroquinoxalines in moderate to good yields and *er* values. Preliminary DFT studies shed light on the role of –OH groups in stabilizing the initially generated *aza*-Breslow intermediates via intramolecular hydrogen bonds. Moreover, photophysical studies on the synthesized dihydroquinoxalines revealed that these molecules can be used for the sensing of various acids and bases.[4] The details of this work will be presented.



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Catalytic, Enantioselective, Directed C2-Functionalization of 3-Aminobenzofurans Using N-Heterocyclic Carbenes

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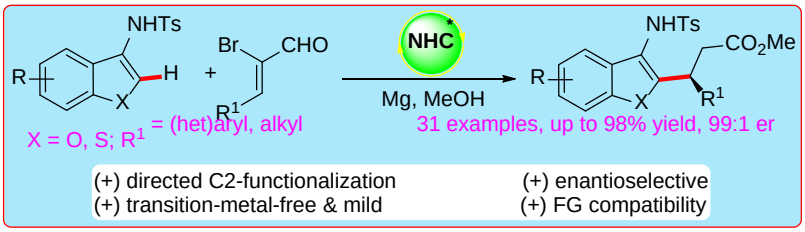
Transition metal catalysed chelation-assisted C-H functionalization of (hetero)arenes is well known in literature for the rapid access to complex molecules from simple starting materials.[1] But transition-metal-free C-H functionalization is limited and will be of high interest. We have developed the N-heterocyclic carbene (NHC) catalysed C2-functionalization of 3-amino benzofurans and benzothiophenes for the synthesis of 2,3-disubstituted heterocyclic compounds in enantioselective fashion.[3] The amine directed C-H functionalization of benzofuran and benzothiophene derivatives was initiated with catalytically generated chiral α,β-unsaturated acylazoliums[4] and proceeds via aza-Claisen rearrangement[5] to deliver the pyridinone derivatives, which undergoes ring-opening catalyzed by Mg to afford the δ-amino acid derivatives with good to excellent yield and enantioselectivity.



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Manganese-Catalysed C-H Activation: A Regioselective C-H Alkenylation of Indoles and other (hetero)aromatics with 4-Hydroxy-2-Alkynoates Leading to Concomitant Lactonization

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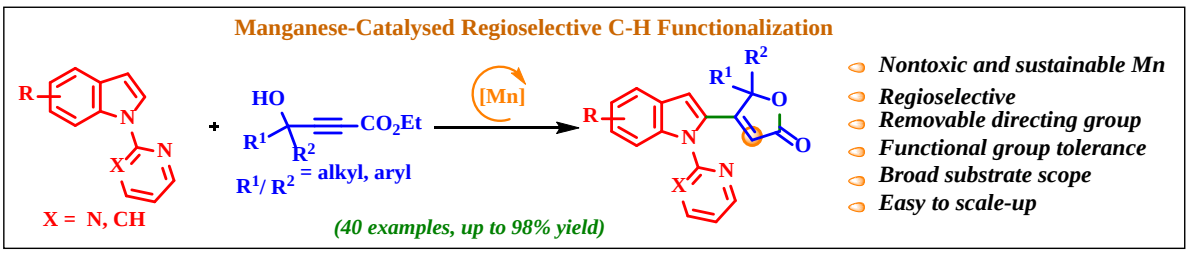
Abstract:

Transition metal-catalyzed C-H bond activation has become a powerful tool for functionalization to obtain complex molecules that find applications in biochemistry, drug discovery, and agrochemicals.[1] Noble transition metal-catalysts of 4d and 5d groups, such as Pd, Rh, Ru, and Ir are widely used for these reactions.[2] Recently, the focus has been moved towards using earth-abundant, inexpensive, less toxic 3d transition metal catalysts such as Co, Cu, and Mn. Among these catalysts, Mn-catalysts in C-H functionalization reactions have received momentum in recent years.[3]

A manganese-catalyzed C-H bond alkenylation of indoles at C2-position with 4-hydroxy-2-alkynoates with concomitant lactonization under removable directing group strategy has been presented. This lactonization strategy exhibits regioselectivity, a broad substrate scope, and a good functional group tolerance furnishing the products in low to high yields. The salient feature of this reaction is the formation of an exclusive single regioisomer with aldehyde and ketone derivatives with bulkier substitution than methyl group at C4 position of alkynoates. Wherein the regioselectivity of the alkyne insertion is controlled by the electronic effect of the ester group as well as increasing the steric bulk at the C4 position of the alkynoates. After the reaction, the directing group has been readily removed to obtain N-H free indole.[4]



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A Comprehensive Mechanistic Analysis on γ-C(sp^3)–H Alkynylation of Aliphatic Carboxamides

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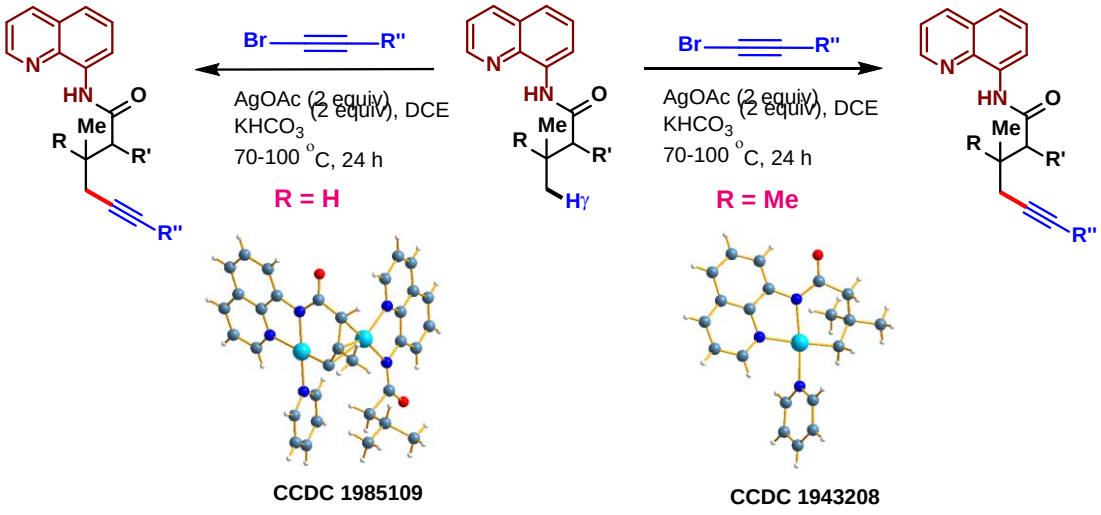
Transition-metal-catalyzed selective C–H functionalization has provided new strategies for synthesizing complex molecular scaffolds.[1] Among these reactions, synthesis of functionalized alkynes deserves a special mention as they can serve as an excellent platform for further diversification.[2] Till now, many methods are developed for the alkynylation of various aromatic C(sp^2)–H bonds, but similar reactions at aliphatic C(sp^3)–H centers are less explored.[3] Here we present an efficient protocol for palladium catalysed γ-selective alkynylation of aliphatic carboxylic acids using 8-aminoquinoline as directing group.[4] This procedure renders high *mono- vs di*-selectivity and shows excellent tolerance to amino-acid analogues. Kinetic studies show that the reaction is first order with respect to both substrate and alkyne, indicating that C–H activation may not be the rate determining step. Further mechanistic studies show that the reaction follows different pathways, in the presence and absence of a β-H atom, involving different intermediates. The C–H activated intermediates in both pathways are isolated and structurally characterized.



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Iterative Arylation of Amino Acids and Aliphatic Amines via δ-C(sp^3)–H Activation: Experimental and Computational Exploration

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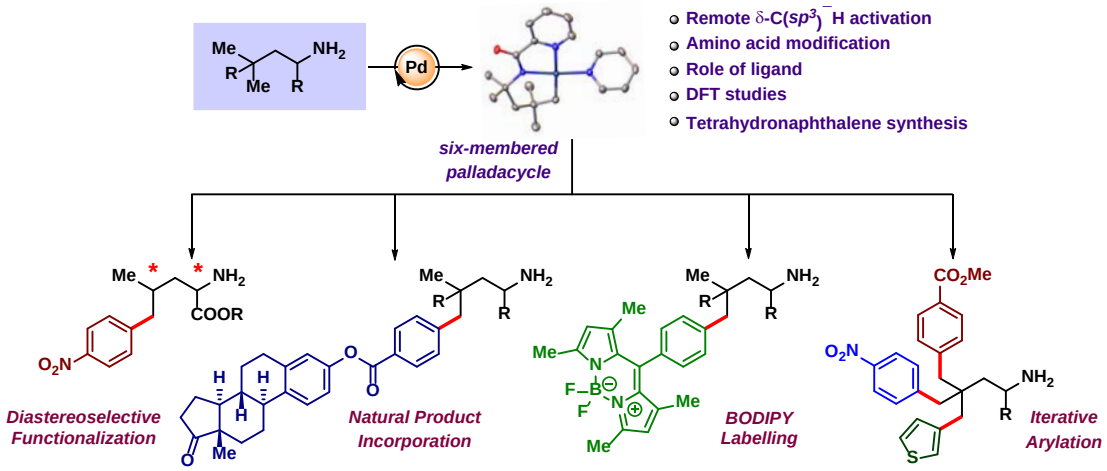
The non-proteinogenic amino acids possess unique biological potential that find application in proteomics and drug discovery. Directed C–H functionalization has been realized as a complementary tool to the traditional approaches for a straightforward access of such non-proteinogenic amino acids; albeit such process is restricted to limited positions (mostly up to γ-position). In this article, we demonstrate the diversification [(hetero)arylation] of amino acids and analogous aliphatic amines selectively at the remote δ-position by tuning the reactivity controlled by ligands. The protocol enables (i) diastereoselective synthesis of δ-arylated leucine; (ii) incorporation of diverse natural products and drugs in amines; (iii) BODIPY labelling of bioactive amines and (iv) iterative (hetero)arylation. The δ-arylated amine products have been utilized for the synthesis of various tetrahydronaphthalene derivatives. Organopalladium δ-C(sp^3)–H activated intermediate has been isolated. Crystallographically characterized intermediate is found to be catalytically and kinetically viable precatalyst. The mechanistic investigations carried out experimentally in conjunction with computational studies shed light on the difference in the mechanistic picture depending on the substrate structure. The multi-faceted aspects of this amine diversification is expected to channelize the pharmaceutical development.



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Ligand Enabled Palladium Catalyzed γ-C(sp^3)-H Arylation of Free Carboxylic Acid

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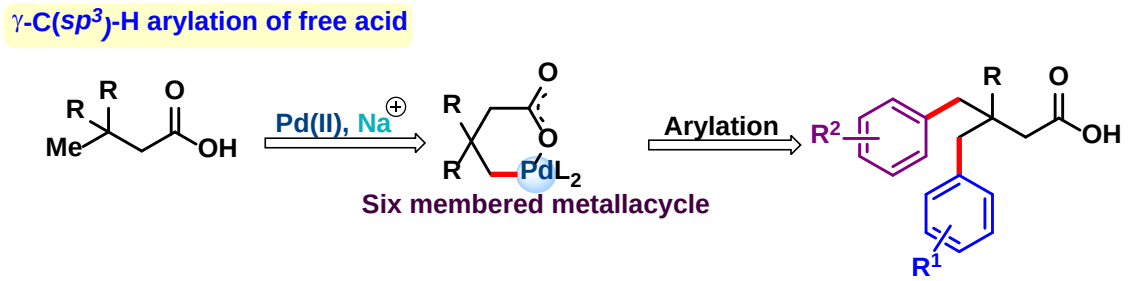
C–H functionalization of aliphatic carboxylic acids without attaching exogenous auxiliary has been so far limited at the proximal β-position[1,2]. Herein, we demonstrate a ligand enabled palladium catalyzed first regioselective distal γ-C(sp^3)–H functionalization of aliphatic carboxylic acids without incorporating an exogenous directing group[3]. Aryl iodides containing versatile functional groups including complex organic molecules underwent the γ-C(sp^3)–H arylation reaction with good to excellent yields. Interestingly, weak coordination of carboxylate group can be further extended for sequential hetero di-arylation.



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Co-ordination assisted distal C–H alkylation of fused heterocycles

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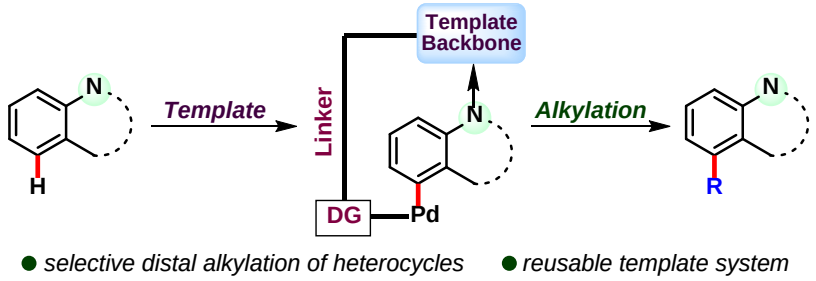

Abstract: Distal C–H bond functionalization of heterocycles remained extremely challenging with covalently attached directing groups (DG). Lack of proper site for DG attachment and inherent catalyst poisoning by heterocycles demand alternate routes for site selective functionalization of their distal C–H bonds. Utilizing non-productive co-ordinating property to hold the heterocycle into the cavity of a template system in a host-guest manner, we report distal C–H alkylation (e.g. C-5 of quinoline and thiazole, C-7 of benzothiazole and benzoxazole) of heterocycles. Upon complexation with heterocyclic substrate, nitrile DG in template directs the metal catalyst towards close vicinity of the specific distal C–H bond of heterocycles. Our hypothesized pathway has been supported by various X-ray crystallographically characterized intermediates.

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Imine as a linchpin approach for distal C(sp^2)–H functionalization

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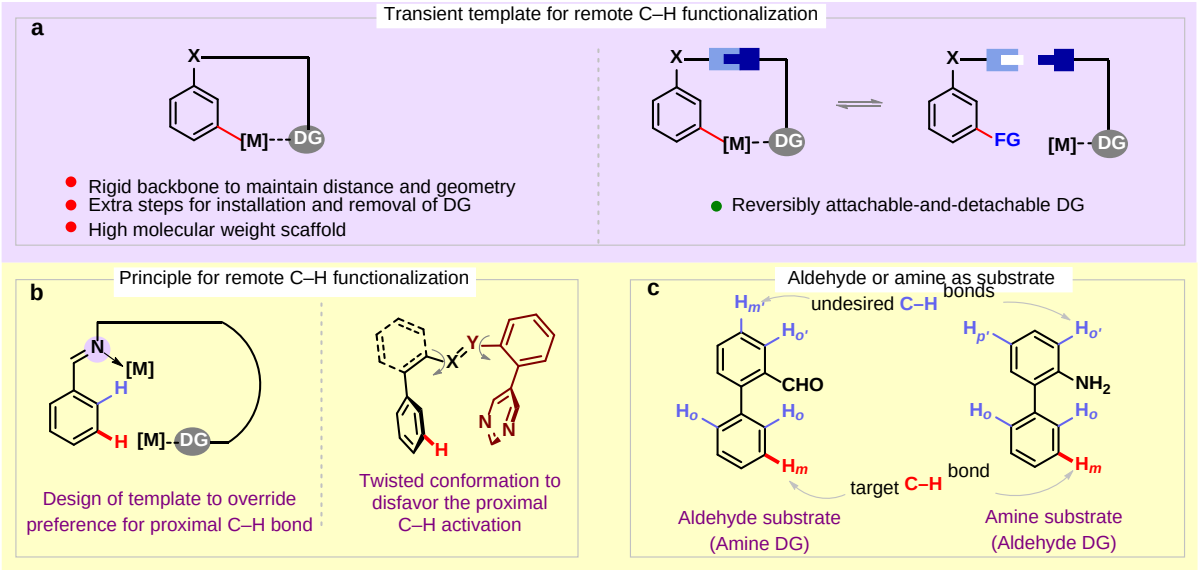
Abstract: Despite the widespread applications of C–H functionalization, controlling site selectivity remains a significant challenge. Covalently attached directing group (DG) served as an ancillary ligand to ensure proximal ortho-, distal meta- and para-C–H functionalization over the last two decades. These covalently linked DGs necessitate two extra steps for a single C–H functionalization: introduction of DG prior to C–H activation and removal of DG post-functionalization. We introduce here a transient directing group for distal C(sp^2)–H functionalization via reversible imine formation. By overruling facile proximal C–H bond activation by imine-N atom, a suitably designed pyrimidine-based transient directing group (TDG) successfully delivered selective distal C–C bond formation. Application of this transient directing group strategy for streamlining the synthesis of complex organic molecules without any necessary pre-functionalization at the distal position has been explored.



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Transition Metal Free Dehalogenative Deuteration/ Hydrodehalogenation of Aryl Halide

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Abstract:

Deuterium incorporation is an important tool for the drug development in pharmaceutical industry and for mechanistic studies in synthetic chemistry.[1,2] Traditional deuteration methods involve the use of costly transition metal catalysts, toxic tin reagents or highly reactive alkyllithium reagents and expensive deuterium source. But, in many cases, precise site selectivity and high deuterium incorporation can't be achieved with these methods. Herein we report a transition metal-free simple and scalable protocol for the dehalogenative deuteration/ hydrodehalogenation of aryl halides. The methodology works at room temperature and involves potassium metal, KO^{t}Bu and DMSO-d6 (or 1,4-dioxane:DMSO) as reagents and phenalenyl as a catalyst.[3] This methodology offers precise site selectivity and high deuterium incorporation and was found to involve a radical mechanism. The single electron transfer mechanism was confirmed via intermediate trapping.

Figure:

References:

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Carbamates: A Selective Directing Groups for C–H Amidation and Alkylation Reactions Under Cp*Co(III)-Catalysis

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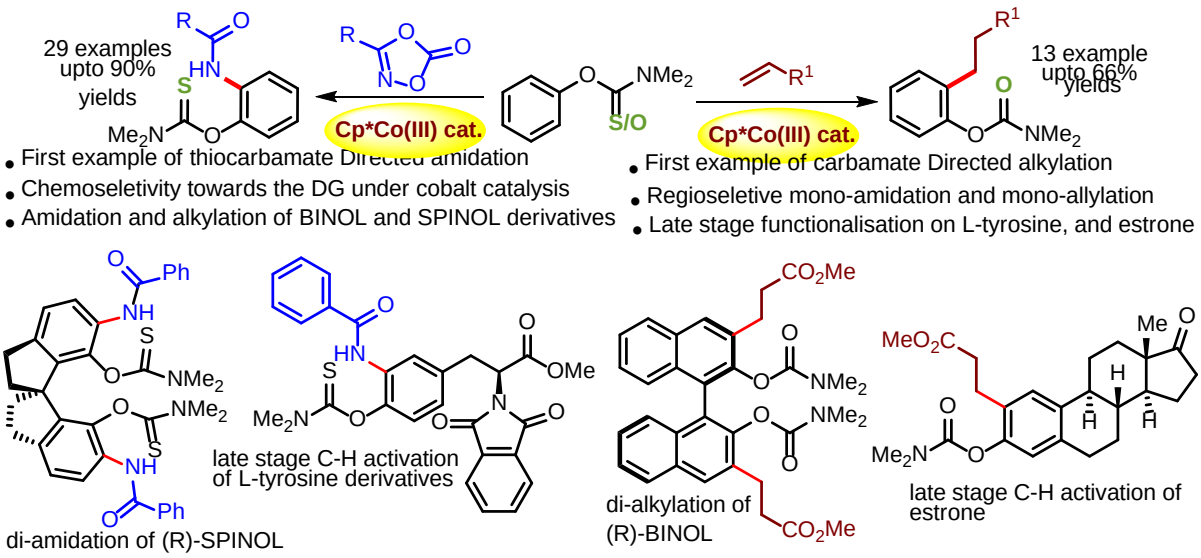
Abstract:

Ortho-functionalization of Phenol derivatives to make C–N bonds and C–C bonds are of immense interest and ideal organic transformations for the construction of numerous biologically active heterocycles, drug molecules, and important synthetic intermediates.[a] An effective strategy development for such transformations have always been a prime interest. To this point, inspired by our continuous effort on cobalt catalyzed C–H bond functionalizations,[b],[c] we have developed the selective reactivity of regioselective amidation and alkylation reactions using thiocarbamtes and carbamates as directing group with the use of stable, high–valent, cost effective cobalt(III) catalysis. The wide scope of this methodology reveals enormous possibility of designing new branch of asymmetric catalyst based on BINOL and SPINOL derivatives. Late stage C-H functionalization of L-tyrosine and estrone was also achieved through our approach. Mechanistic study shows a Base Assisted Intermolecular Electrophilic Substitution mechanism is operative here.



Scheme 1. Thiocarbamate and Carbamate Directed Amidation and Alkylation

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