Modern Aspects of Green and Sustainable Chemistry 2026

MAGSuC-2026

January 27-30, 2026

SHIV NADAR
INSTITUTION OF EMINENCE DEEMED TO BE
UNIVERSITY
DELHI NCR

SCHOOL OF
NATURAL
SCIENCES

CONTENT

About Shiv Nadar Institution of Eminence & department of chemistry

Shiv Nadar Institution of Eminence (SNIOE), Deemed to be University, is a comprehensive, multidisciplinary, research-focused, and student-centric institution that is bringing a paradigm shift in higher education in India through its innovative curriculum, interdisciplinary focus, and cross-disciplinary thinking across a wide range of disciplines. The University is building an ecosystem of knowledge to promote recognition of the interconnectedness of ideas, systems, and environments, nation- and world-wide. The University has 5 Schools, 18 Departments, and 6 Research Centers engaged in teaching, practice, and research in disciplines as diverse as Engineering, Humanities & Social Sciences, Management, Natural Sciences, Art, Design, Performing Arts, Communication, and Extended Education & Professional Development. The Schools offer Bachelor, Master, and Doctoral degrees along with multidisciplinary curriculum to enable students in exploring subjects and disciplines that may be widely different from their chosen Majors – Learning is choice-driven.

- The University received Institution of Eminence Deemed to be University status by the Government of India in August 2022.
- In the **NIRF** (Government's National Institutional Ranking Framework), SNIoE has been the youngest institution in the 'top 100' *Overall* list, and the score has been rising steadily. SNIoE ranked 61 in the *University* category, and 94 '*Overall*' in NIRF 2022.
- The University has been accredited with **'A' Grade** by the National Assessment and Accreditation Council **(NAAC)**, valid for a period of 5 years from 26 November 2019.
- SNIoE is also among a select group of green-field institutions in the country, which were awarded the prestigious **Atal Incubation Center** grant by the Niti Aayog, Government of India, in the very first round in 2017.
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About the Chemistry Department

The Department is committed to pursuing research on fundamental and applied problems through scientific inquiry, and stimulating the development of innovative interdisciplinary research programs around key areas of excellence. The immediate mission of Chemistry Department is to:

- Contribute to advancing and disseminating chemical knowledge through educational programs, internationally reputed publications and translating research as innovative patents.
- Devise robust and novel solutions to address the needs of society by promoting research in chemical and interdisciplinary projects.
- Train undergraduate, graduate students and research fellows to transform them future independent scientists to serve the needs of society, academia and industries.

Our vision is to make the world a better place through societal-impact cutting-edge research and innovation at Shiv Nadar Institution of Eminence, Deemed to be University.

Research Infrastructure

Our chemistry labs are equipped with fume-hoods, Schlenk lines, eyewash stations and safety showers. Lab facilities include advanced analytical instruments such as EPR, AFM, Flash Chromatography, Gas Chromatography with MS, Gel Permeation Chromatography, HPLC (Prep & Analytical), FPLC, NMR, LCMS-qToF, MALDI-ToF, DSC, TGA, Single-crystal X- ray Diffractometer, Electrochemical Analyzer, Fluorimeter, TCSPC, Polarimeter, UV-visible, High-resolution FTIR, Raman Spectrometers, Microwave Reactor, Inverted Microscope, Fluorescent Microscope, Hot-stage Polarized Microscope, Ferroelectric-Piezoelectric- Pyroelectric test system, Bio-safety Cabinets, CO2 Incubators, Shaker Incubators, Glove box, Multimode Plate Reader, Electroporator, Deep freezer, Cell Counter etc.

Computational facilities that include a high-performance IBM cluster (“Magus”) having 8064 cores along with two nodes with GPGPU processors, delivering a theoretical peak performance of ~320TF. Additionally, several Linux workstations are used for teaching as well as research purposes. Software for bioinformatics and cheminformatics, molecular modeling, molecular dynamics, quantum chemistry, data analysis, and statistical learning is also available.

Our library, housed in a modern 5-storey building, provides online access from anywhere on campus to a large number of electronic journals and databases, including APS, AIP, ACS, RSC, AMS, SIAM, Springer, Elsevier, Wiley, and Nature journals, in addition to various books, e-books, and other learning resources.

Please visit the following links to know more about our research laboratories and facilities. https://chemistry.snu.edu.in/research/laboratories

https://snu.edu.in/research/facilities

Our Motto: *To Provide the Opportunity of Learning Through Research Experience*

Experiential and Effective Learning*: Teacher & Student Ratio (1:9) and a Research Ecosystem*

We Offer*: Core and Elective courses that are highly relevant to the current scenario*

B.Sc. (Research) | M.Sc. (Research) | Integrated M.Sc.-Ph.D. | Ph.D.

ABOUT THE CONFERENCE

The growing concern over our depleting environment has prompted a global awareness about its preservation and sustainability. Numerous facets of our daily life, such as households, transportation, hospitality, consumer industries, food and beverages, life care, etc., are presently being scrutinized and the corresponding processes are being improved to make them ecologically compatible.

To protect the environment, the scientific communities from academia and industry have discovered, and are still developing, strategies for performing sustainable organic synthesis. Based on this assessment, we have organized this scientific congregation consisting of 1.5 days of workshop and 2.5 days of conference, aiming to discuss and highlight numerous Green and Sustainable organic processes, as well as technologies, from students, academicians, and industry personnel involved in this research area.

CONFERENCE THEME

- **Covalent Organic Frameworks**
- **Electrocatalysis**
- **Homogeneous Asymmetric Catalysis**
- **Medicinal Chemistry**
- **Transition Metal Catalysis**
- **Supramolecular Chemistry & Chemical Biology**
- **Computational Catalysis**

PROGRAMME SCHEDULE OF THE WORKSHOP

SHIV NADAR INSTITUTION OF EMINENCE DEEMED TO BE UNIVERSITY DELHI NCR | SCHOOL OF NATURAL SCIENCES

Day 1: January 27, 2026 (Tuesday)	
REGISTRATION & BREAKFAST (8:30-9:45)	
INAUGURATION (G Block Auditorium)	
09:45-10:30	Welcome by Vice-chancellor/Dean SoNS Head of the Department/ Convenor of Organizing Institution, MAGSuC – 2026
Workshop (G 206)	
WORKSHOP SESSION-I (Chairperson: **Prof. Gremaud Ludovic**)	
10:30-12:00	Drug Discovery and Process Development *Novartis, India or Switzerland*
Lunch- G Block (12:00-14:30)	
WORKSHOP SESSION-II (Chairperson: **Dr. Naiwrit Karmodak**)	
14:30-16:00	Dynochem ***Dr. Sanket Salgaonkar**, Mettler Toledo India Pvt. Ltd.*
Tea/Coffee Break (16:00-16:30)	
WORKSHOP SESSION-III (Chairperson: **Prof. Subhabrata Sen**)	
16:30-18:00	**Process Safety** ***Prof. Dr. Andreas Zogg**, School of Life Science FHNW, Switzerland (online)*

End of the Day 1 (Dinner @ G Block from 19:30 to 22:00)

PROGRAMME SCHEDULE OF THE CONFERENCE

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SCHOOL OF NATURAL SCIENCES

Day 2: January 28, 2026 (Wednesday)	
Breakfast G-Block (8:00-9:00)	
WORKSHOP SESSION-IV G206 (Chairperson: **Dr. Kshatresh Dutta Dubey**	
9:00-10:30	Application of Machine Learning in Drug-Discovery ***Dr. Aditya Padhi***, *IIT BHU, India*
Tea/Coffee Break (10:30-10:45)	
WORKSHOP SESSION-V (Chairperson: **Dr. Arnab Ghosh**)	
10:45-11:30	Flow Chemistry ***Sandeep Mandke***, *Buchi Glass, India*
WORKSHOP SESSION-VI (Chairperson: **Dr. Biswajit Guchhait**)	
11:30-13:00	Sustainable Crop Protection Discovery ***Dr. Chandan Dey***, *BASF India*
WRAP-UP WORKSHOP (13:00-13:15)	
Lunch G-Block (13:15-14:30)	
WELCOME & CONFERENCE REGISTRATION (G-Block Auditorium)	
14.30-15.00	Welcome by Dean of School of Natural Science or VC/ Convenor of Organizing Institution, MAGSuC – 2026
	SESSION-I (Chairperson: **Prof. Vijay Kumar**)
15:00-16:00	Plenary Lecture (PL-01): ***Prof. Junji Nakamura***, *Kyushu University, Japan* Title: *Proposal of Methanol Society -The Role of Catalyst Research*
	Tea/Coffee Break (16:00-16:30)
	SESSION-II (Chairperson: **Dr. Santanu Ghosh**)
16:30-17:15	Keynote Lecture (KNL-01): ***Prof. Santanu Mukherjee***, *IISc Bangalore, India* Title: *Symmetry Breaking Routes to Natural and Unnatural Ladderanes*
17:15-17:50	Invited Lecture (IL-01): ***Dr. Vishal Dhavale, CSIR-CECRI***, *India* Title: *Electrocatalyst and Electrolyte Engineering for Energy Applications*
17:50-18:10	Short Invited Lecture (SIL-I): ***Dr. Abhijit Dan***, *Maulana Abul Kalam Azad University of Technology, India* Title: *Ultra-Stable Liquid Crystal-In-Water Emulsions As Optical Biosensors*

End of the Day 2 (Gala Dinner at **Stellar Gymkhana** 19:30 to 23:00)

Day 3: January 29, 2026 (Thursday)	
Breakfast (8.00-9.00)	
SESSION-III (Chairperson: **Dr. Ajoy Kapat**)	
9:00-10:00	Plenary Lecture (PL-02): ***Prof. Erick M. Carreira,*** *ETH Zurich, Switzerland*
10:00-10:35	Invited Lecture (IL-02): ***Dr. Prakash P. Neelakandan****, INST Mohali, India* Title: *Broadening the Functional Scope of Imino(Boron) Compounds in Energy-Related Applications*
Tea/Coffee Break (10:35-11:00)	
SESSION-IV (Chairperson: **Dr. Debdas Ray**)	
11:00-12:00	Plenary Lecture (PL-03): ***Prof. Rahul Banerjee****, IISER Kolkata, India* Title: *Reticular Chemistry: Covalent Organic Framework Porous Crystalline Nitrogen Doped Graphite*
12:00-13:00	Plenary Lecture (PL-04): ***Prof. D. Srinivas Reddy,*** *IICT Hyderabad, India* *Title: Efforts in Drug Discovery through Druggable Scaffold of Natural Products and Process Development of a Lifitegrast Intermediate with Low Carbon Footprint*
Photo Session & Lunch-Poster Session (13:00 -14:00)	
SESSION-V (Chairperson: **Prof. Parthapratim Munshi**)	
14.00-14.45	Keynote Lecture (KNL-02): ***Prof. Murugavel****, IIT Bombay, India* Title: *Metal Phosphate Molecules and Materials for Energy Transition*
14:45-15:20	Invited Lecture (IL-03): ***Dr. Garima Jindal,*** *IISc Bangalore, India* Title: *Dirhodium Catalysts: From Mechanistic Aspects to Synthesis to Application*
15.20-15.55	Invited Lecture (IL-04): ***Dr. Chinmoy Hazra****, IIT Delhi, India* Title*: Regioselective, Non-Directed C–H Functionalization of Small Molecules via Brønsted Acid Catalysis*
Tea/Coffee Break (15:55-16:15)	
SESSION-VI (Chairperson: ***Dr. Bappaditya Gole***)	
16:15-17:00	Keynote Lecture (KNL-03): ***Prof. Kana M. Sureshan,*** *IISER TVM, India* Title: Topochemistry for Solving Challenges in Poly Synthesis
17:00-17:35	Invited Lecture (IL-05): ***Prof. Biplab Maji****, IISER Kolkata, India* Title: *Expanding the Toolbox of Catalysis: From Light-Driven Dearomatization to Remote C–H Functionalization to Polymer Upcycling*
17:35-18:10	Invited Lecture (IL-06): ***Dr. Amit Kumar Mondal,*** *INST Mohali, India* *Title*: Spintronics and Chirality: Spin Selective Electron Transport through Chiral Molecules

18:10-18:20	Flash Talk (FL-01): ***Dr. Arijit Mallick,*** *JNU, India* Title: *Metal-Organic Frameworks (MOFs) for CO_2 Capture from Air*
End of the Day 3 (Dinner @ G Block from 7:30 to 10:00 PM)	

Day 4: January 30, 2026 (Friday)	
Breakfast (8.00-9.00)	
SESSION-VII (Chairperson: Dr. **Basab Bijayi Dhar**)	
9:00-9:45	Keynote Lecture (KNL-04): ***Prof. Partha Sarathi Das****, IIT-ISM Dhanbad, India* Title: *Expanding Discovery Chemistry Toolbox: From Concept to Practice*
9:45-10:20	Invited Lecture (IL-08): ***Prof. Dr. Roger Marti****, HEIA-FR, Switzerland* Title: *Single-Atom Pd Catalysts for Sonogashira Coupling: Bridging Green Metrics, Ligand Design, & Scale-Up*
10:20-10:30	Flash Talk (FL-02): ***Dr. Priyabrata Ghana****, IIT Gandhinagar, India* Title: *Transforming Dinitrogen into Trisilylamine via Homogeneous Titanium Catalysis*
Tea/Coffee Break (10:55-11:15)	
SESSION-VIII (Chairperson: **Dr. Santosh K. Singh)**	
11.15-12.00	Keynote lecture (KNL-05): ***Prof. Nitin Patil****, IISER Bhopal, India* Title: *Enantioselective Gold Redox Catalysis*
12:00-12:35	Invited Lecture (IL-08): ***Dr. Kotaro Takeyasu***, University of Hokkaido, Japan Title: *Hybrid Thermochemical–Electrochemical Catalysis Enabled by Mixed Potentials: Design of Green CO_2 Conversion Reactions*
12:35-12:45	Flash Talk (FL-04): ***Dr. Debajit Maiti****, Krea University, India* Title: *Electrooxidative Divergent Halocyclizations of Ambident Amides*
12:45-12:55	Flash Talk (FL-05): ***Dr. Snehanshu Patra****, Eliteck Industries Pvt Ltd, India* Title: *Transforming The Chemically Impossible Into Scalable Reality Via Electrochemistry.*
Photo session G Block Entrance (12:55-13:15)	
Lunch & Poster Session (13:15 To 14:15)	
SESSION-IX (Chairperson: **Dr. Tatini Rakshit**)	
14:15 -14:50	Invited Lecture (IL-9): ***Prof. Sandeep Kaur***, University of Delhi**,** India Title: *Hydrogen Evolving Mono-nuclear Complexes with Carefully Positioned Ligands.*
14:50 - 15:25	Invited Lecture (IL-10): ***Prof. Bimlesh Lochab****, Shiv Nadar Institution of*

	Eminence, India Title: *Circular Thermosets: Transforming Concepts into Sustainable Solutions.*
15:25-16:00	Invited Lecture (IL-11): ***Dr. Amit Kumar***, *IIT Patna**,** India* Title: *From Simple to Complex: Synthesis of Key Heterocyclic Compounds*
16:00-16:20	Short Invited Lecture (SIL-02): ***Dr. Shiva Prasad***, *University of Delhi, India* Title: *Aminocatalytic Asymmetric Remote Functionalization to Access Biologically Potential Scaffolds*
16:20-16:55	**Valedictory Session & End of Conference**

List of Plenary, Key Note, Invited & Flash Talks

Serial No	Name of the Participant	Name of the Institute	Lecture Number
		Plenary Lecture (PL)	
1	**Prof. Junji Nakamura**	Kyushu University, Japan	**PL1**
2	**Prof. Erick M Carreira**	ETH Zurich, Switzerland	**PL2**
3	**Prof. Rahul Banerjee**	IISER Kolkata, India	**PL3**
4.	**Prof. D. Srinivas Reddy**	IICT Hyderabad, India	**PL4**
		Keynote Lecture (KNL)	
1.	**Prof. Santanu Mukherjee**	IISc Bangalore, India	**KNL 1**
2.	**Prof. Murugavel**	IIT Bombay, India	**KNL2**
3.	**Prof. Kana M Sureshan**	IISER TVM, India	**KNL3**
4.	**Prof. Partha Sarathi Das**	ISM Dhanbad, India	**KNL4**
5.	**Prof. Nitin Patil**	IISER Bhopal, India,	**KNL5**
		Invited Lecture (IL)	
1.	**Dr. Vishal Dhavale**	CSIR-CECRI, India	**IL01**
2.	**Dr. Prakash P. Neelakandan**	INST Mohali, India,	**IL02**
3.	**Dr. Garima Jindal**	IISc Bangalore, India	**IL 03**
4.	**Dr. Chinmoy Hazra**	IIT Delhi, India	**IL04**
5.	**Dr. Biplab Maji**	IISER Kolkata, India	**IL05**
6.	**Dr. Amit Kumar Mondal**	INST Mohali, India	**IL06**
7.	**Prof. Dr. Roger Marti**	HEIA-FR, Switzerland	**IL07**
8.	**Dr. Kotaro Takeyasu**	University of Hokkaido, Japan	**IL08**
9.	**Prof. Sandeep Kaur**	University of Delhi, India	**IL09**

10.	**Prof. Bimlesh Lochab**	Shiv Nadar Institution of Eminence, India	**IL10**
11.	**Dr. Amit Kumar**	IIT Patna, India	**IL11**
		Short Invited Talk (SIL)	
1.	**Dr. Abhijit Dan**	Maulana Abul Kalam Azad University of Technology, India	**SIL-01**
2.	**Dr. Shiv Prasad**	University of Delhi, India	**SIL-02**
		Flash Talk (FT)	
1.	**Dr. Arijit Mallick**	JNU, India	**FT01**
3.	**Dr. Ghana**	IIT Gandhinagar, India	**FT 03**
4.	**Dr. Debajit Maiti Dr.**	Krea University, India	**FT 04**
5.	**Snehanshu Patra**	Eliteck Industries Pvt Ltd, India	**FT 05**

List of Participants for The Poster Presentation

Serial No	Name of the Participant	Name of the Institute	Poster Number
1.	**Ajay B. Shelke**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P01**
2.	**Amar Jeet Yadav**	Indian Institute of Technology (BHU) Varanasi	**P02**
3.	**Amit Kumar**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P03**
4.	**Anil Kumar U**	Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India	**P04**
5.	**Ashirwad Divedi**	Babasaheb Bhimrao Ambedkar University, Uttar Pradesh	**P05**
6.	**Asrar Ahmad**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P06**
7.	**Azzharuddin Sardar**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P07**
8.	**Chaithra Rajeev**	CSIR-Central Electrochemical Research Institute-Madras Unit, CSIR Madras	**P08**
9.	**Devang Shukla**		**P09**
10.	**Dhanyashree Das**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P10**
11.	**Diksha**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P11**
12.	**Dipti R. Panigrahi**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P12**
13.	**Garvit Gupta**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P13**
14.	**Haya Khan**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P14**
15.	**Kaito Homma**	Hokkaido University	**P15**
16.	**Kajal Uphade**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P16**
17.	**Lokesh Gupta**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P17**
18.	**Mansi Gupta**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P18**

19.	**Mridul Jain**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P19**
20.	**Naga M. R. Vampugani**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P20**
21.	**Neha Kundara**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P21**
22.	**Nitin Kumar Tyagi**	Technical University of Eindhoven, Netherlands	**P22**
23.	**Pranjit Barman**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P23**
24.	**Prashant B. Singh**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P24**
25.	**Keerthipati P.K.**	National Sun Yat-sen University, Taiwan	**P25**
26.	**Rabban**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P26**
27.	**Rafique Sanukhan**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P27**
28.	**Rajeshwari Avhad**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P28**
29.	**Roopam Pandey**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P29**
30.	**Saumya Singh**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P30**
31.	**Shagun Singh**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P31**
32.	**Shouvik Mete**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P32**
33.	**Shweta Singh**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P33**
34.	**Srishti Ahlawat**	Jawaharlal Nehru University, New Delhi, India	**P34**
35.	**Subhankar Bera**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P35**
36.	**Vaibhav Cholke**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P36**
37.	**Vasanthapandiyan M**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P37**
38.	**Yashika Tyagi**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P38**
39.	**Sarban Kumar Yadav**	Shiv Nadar Institution of Eminence, Delhi-NCR	**P39**
40.	**Amar Jeet Yadav**	Indian Institute of Technology (BHU) Varanasi	**P40**

Bio-Sketch

Junji Nakamura
Research Professor

Kyushu University International Institute for Carbon-Neutral Energy Research (I2CNER), Mitsui Chemicals, Inc. – Carbon Neutral Research Center (May 2023- now) Emeritus Professor in University of Tsukuba
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Website: https://nakamurajunji700.wixsite.com/nakamura-lab

Professional Experience

Research Professor, Kyushu University, International Institute for Carbon-Neutral Energy Research (I2CNER) (April 2023–Present), Professor, Kyushu University, I2CNER (May 2022–March 2023), Professor, Department of Materials Science, University of Tsukuba (June 2006–April 2022), Associate Professor / Lecturer, University of Tsukuba (1990–2006), Postdoctoral Fellow, University of Washington, USA (1989–1990), Postdoctoral Fellow, Indiana University, USA (1988–1989)

Awards & Honors

Award of the Catalysis Society of Japan (1993), Fellow of the Surface Science Society of Japan (2016), Surface Science Society Award (2017), Commendation for Science and Technology by MEXT, Japan (2018), Catalysis Society of Japan Award (Academic Field) (2018), Education Award, Catalysis Society of Japan (2023)

Membership

The Chemical Society of Japan, Catalysis Society of Japan, The Surface Science Society of Japan (Fellow), American Vacuum Society (AVS), American Chemical Society (ACS), CHEMRAWN, IUPAC (2024–2027)

Research

Junji Nakamura has carried out a unique fusion of surface science and catalytic chemistry to elucidate solid-state catalytic mechanisms at the atomic and electronic levels. By constructing well-defined single-crystal model catalysts and quantitatively correlating their activity with real powder catalysts, he has revealed active sites and reaction mechanisms with unprecedented precision. His research seamlessly connects fundamental surface science, theoretical calculations, and catalyst design, covering heterogeneous catalysts such as Cu-based methanol synthesis catalysts, fuel cell catalysts, nitrogen-doped carbon catalysts, and graphitic carbons. Nakamura's representative researches are establishing the Cu–Zn alloy active-site model for methanol synthesis catalysts, discovering a rare Eley–Rideal mechanism for formate formation (Nature Chemistry, 2019), and resolving the long-standing controversy on nitrogen-doped carbon catalysts by identifying pyridinic nitrogen as the active site for oxygen reduction, reported in Science (2016), now one of the most cited catalyst papers worldwide.

Plenary Lecture (PL -1)

Proposal of Methanol Society -The role of catalyst research -

Junji Nakamura
International Institute for Carbon-Neutral Energy Research, Kyushu University,
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Abstract

Scientific research has confirmed that climate change is driven by anthropogenic CO_2 emissions. To combat this, urgent measures are needed to capture CO_2 at emission sources and implement renewable energy efficiently worldwide, requiring global cooperation among scientists, engineers, and policymakers. A key solution is converting captured CO_2 into an energy carrier. Among various options, methanol emerges as the most suitable carrier. This conclusion is based on 30 years of dedicated research into methanol synthesis catalysts from CO_2. Catalytic chemistry plays a critical role in producing sustainable energy fuels, replacing cheap fossil fuels.

In this presentation, I will discuss why methanol is an effective energy carrier. True innovation involves technology that can be utilized in any country, including those with limited resources. Methanol synthesis from CO_2 is feasible globally, using inexpensive copper as a catalyst. The energy required for this process at 250°C and 50 atm is relatively low. Additionally, methanol offers advantages such as easy handling, suitability as fuel for internal combustion engines and fuel cells, and utility in chemical synthesis processes like the MTO process. Above all, it is an ideal energy carrier that facilitates CO_2 recycling.

I also introduce model catalyst studies of methanol synthesis over Cu/ZnO [1-4]. In the 1990s, we have reported that CuZn alloy sites form active sites in model catalysts using Cu(111) with deposited Zn [4]. It has been found that that the CuZn site promotes the hydrogenation of formate ($HCOO_a$) on Cu, while Cu sites play a role to produce formate from CO_2 and adsorbed H_a via Eley-Rideal type mechanism. When the bending mode of the linear CO_2 molecule is excited, its reactivity as an acid increases due to the reduction in the LUMO level. This allows CO_2 to react with hydrogen on the Cu surface without the need to heat the catalyst [1]. Understanding the mechanism of heterogeneous catalysis is equivalent to creating a potential diagram of the reaction intermediates. A potential diagram for methanol synthesis from CO_2 using Cu-based catalysts is being created [2].

Keywords: Carbon neutrality, Methanol, catalyst, Cu/ZnO, CO_2

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Bio-Sketch

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Professional Experience

- **2021- till date:** Professor, Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata
- **2017-2021:** Associate Professor, Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata
- **2011-2017:** Scientist E-1, CSIR-National Chemical Laboratory, Pune, India
- **2008-2011:** Scientist C, CSIR-National Chemical Laboratory, Pune, India

Academic

- **2006-2008:** Research Associate, UCLA-Los Angeles, USA
- **2000-2006:** Research Scholar, University of Hyderabad, India

Awards & Honors

- Clarivate Highly Cited Researcher (in Chemistry) since 2019-
- Alexander von Humboldt Foundation's Ambassador Scientist (India) 2025-
- Fellow of the Indian Academy of Sciences (2021)
- Fellow of the Indian National Science Academy (2025)
- Associate Editor and Editorial Board member of *J. Am. Chem. Soc.,* [2021-till date]
- Recipient of the Shanti Swarup Bhatnagar Prize in Chemical Sciences for the year 2018.
- Recipient of the Swarna Jayanti Fellowship in Chemical Sciences for the year 2016-2017.
- Recipient of the B. M. Birla Science Prize in Chemistry for the year 2015.
- Recipient of Alexander von Humboldt Research Fellowship Programme for Experienced Researchers 2016
- Recipient of Thomson Reuters Research Excellence-India Citation Awards, 2015
- Recipient of NASI-SCOPUS Young Scientist Award in Chemistry, 2014
- Associate Editor and Editorial Board member of *Chemical Science* [2018-2020]
- Associate Editor and Editorial Board member of *CrystEngComm* [2011-2018]
- Recipient of CSIR- Young Scientist Award 2011
- Recipient of NASI- Young Scientist Platinum Jubilee Award 2011

Plenary Lecture (PL -3)

Reticular Chemistry: Covalent Organic Frameworks to Porous Crystalline Nitrogen Doped Graphite

Rahul Banerjee *

[a]Professor/Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur Campus, Mohanpur 741 246

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Abstract

Covalent Organic Frameworks (COFs) represent a novel class of highly porous, crystalline polymers with uniformly ordered pore channels. Despite their extensive use for storing various molecular species such as gases, nanoparticles, enzymes, and drugs, the potential of their ordered pore channels for molecular separation still needs to be utilized. A significant obstacle is fabricating COF particles into self-standing, stable membranes. Beyond processability, other significant barriers to the real-world application of COFs include (i) chemical stability, (ii) complex synthesis procedures, and (iii) scalability. In this context, we have successfully addressed the chemical stability issue by synthesizing β-ketamine-based frameworks. Furthermore, recent advances in Reticular Chemistry have led to the development of Covalent Organic Nanotubes (CONTs), which extend the principles of COF design into one-dimensional architectures. These CONTs, formed by linking molecular building blocks in a reticular fashion, offer unique properties such as tunable pore sizes and enhanced stability, making them promising candidates for molecular separation, catalysis, and nanofiltration applications. Integrating reticular chemistry in one dimension opens new avenues for designing functional materials with precise control over their structural and chemical features. Our findings highlight that COMs and CONTs have significant potential to address some of the world's most challenging separation problems, including wastewater treatment and drug recovery in the pharmaceutical industry.

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Bio-Sketch

D. Srinivasa Reddy
Director

Indian Institute of Chemical Technology (IICT)
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D. Srinivasa Reddy obtained his PhD in Synthetic Organic Chemistry under the guidance of Prof. Goverdhan Mehta from the University of Hyderabad. Later postdoctoral work under Prof. Sergey A. Kozmin followed with Prof. Jeffrey Aubé at the University of Kansas, USA. Before embarking on his journey in Academia at CSIR-NCL, Dr Reddy worked in the industry for seven years Dr. Reddy's Laboratories and TATA Advinus. During that period, he gained experience in leading various drug discovery programs, particularly, in the area of metabolic disorders. Two projects that he led at Dr Reddy's and TATA Advinus went through the full cycle of hit identification, hits-to-leads and lead optimization phases. Under his project leadership, the drug candidate LIK066 was discovered in a collaboration program between Novartis & Advinus which was in advanced human clinical trials (Phase II). During his tenure in CSIR-NCL, his team out-licensed patent/technology (two nos.). During his tenure as a director of CSIR-IIIM, Jammu & Kashmir, he played a key role in popularizing Purple Revolution for the benefit of farmers in Jammu & Kashmir and DCGI approval of Hydroxyurea drug in India for Sickle cell anaemia patients. Presently he is the Director of CSIR-IICT, Hyderabad where the institute focus is on healthcare, chemicals, energy and environment.

Research Interests

Total Synthesis of Natural Products; Medicinal Chemistry; Process Development and Drug Discovery

Awards and Honours

- J. C. Bose National Fellowship by SERB, DST, Govt. of India
- Shanti Swarup Bhatnagar Prize in chemical sciences
- Fellow of the Indian National Science Academy, India (INSA)
- Fellow of the Indian Academy of Sciences, India (FASc)
- Fellow of the National Academy of Sciences, India (FNASc)
- NASI-Reliance Industries Platinum Jubilee Award - physical sciences
- Sun Pharma Research (Ranbaxy) Award - pharmaceutical sciences
- OPPI Scientist Award for contributions in pharmaceutical sciences
- Nominated to the scientific body of Indian Pharmacopoeia, Govt. of India
- CRSI Bronze Medal in chemical science
- CDRI Award for Excellence in drug discovery research - chemical science

Plenary Lecture (PL -4)

Efforts in Drug Discovery through Druggable Scaffolds of Natural Products and Process Development of a Lifitegrast Intermediate with Low Carbon Footprint

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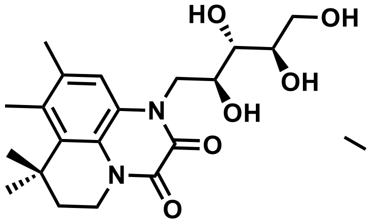
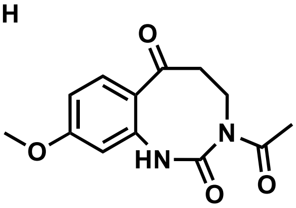
Abstract

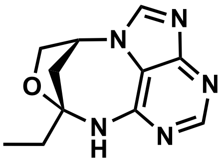
Our research group focuses on total synthesis of biologically active compounds and medicinal chemistry with an aim of discovering drugs. We have accomplished the synthesis of more than 50 natural products which include cell-adhesion inhibitors, anti-bacterial, anti-malarial, anti-inflammatory, anti-cancer agents, and CNS agents sex pheromones and insect repellents. Here, I will be discussing on a couple of case studies from my research group such as Hunanamycin, Peganutonin, Cyclopeltain and related ones. We have accomplished synthesis, prepared libraries of compounds and identification of leads for developing potential drugs. In the later part, Scalable synthesis of benzofuran-6-carboxylic acid, a key fragment of an ophthalmic drug Lifitegrast The life cycle analysis comparison of existing and present routes indicated roughly that the present route leaves less carbon footprint.



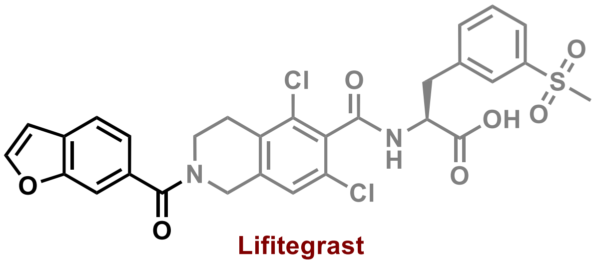
Hunanamycin A
Antibacterial



Peganutonin A
(Putative structure)
Antiviral



Cyclopeltain B
Antiinflammatory



Lifitegrast
drug used for treating dry eye syndrome

Bio-Sketch

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Bangalore

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Professional Experience

- Professor at the Department of Organic Chemistry, IISc Bangalore (since 12/2021)
- Associate Professor at the Department of Organic Chemistry, IISc Bangalore (12/2015 – 12/2021)
- Assistant Professor at the Department of Organic Chemistry, IISc Bangalore (04/2010 – 12/2015)

Academic

- Postdoctoral Associate at Harvard University, USA with Prof. E. J. Corey (06/2008 – 02/2010)
- Postdoctoral Associate at MPI für Kohlenforschung, Mülheim, Germany with Prof. Benjamin List (06/2006 – 05/2008)
- PhD (Organic Chemistry) at Universität zu Köln, Germany with Prof. Albrecht Berkessel (2006)
- MSc (Chemistry) at Indian Institute of Technology, Kanpur, India (2002)

Awards & Honors

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

Membership:

- Fellow of the Royal Society of Chemistry, London, UK (FRSC)

Keynote Lecture (KNL-1)

Symmetry Breaking Routes to Natural and Unnatural Ladderanes

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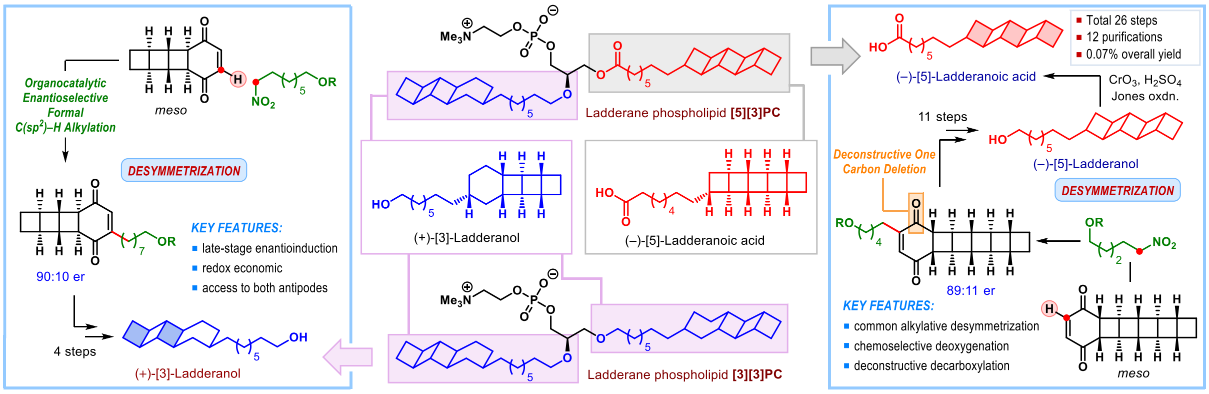
Abstract

Breaking symmetry to generate asymmetry, commonly termed *desymmetrization*, is a remarkably powerful strategy for building molecular complexity. During the past few years, we have developed a number of organocatalytic enantioselective desymmetrization reactions including formal C(sp^2)–H alkylation[1] and *de novo* construction of (hetero)arenes.[2] We subsequently applied these reactions to the enantioselective synthesis complex targets.

Naturally occurring ladderane phospholipids represent such target, which provided us with the motivation to develop some of these enantioselective desymmetrization reactions. This talk will focus on the application of our desymmetrizing C(sp^2)–H alkylation reaction to [3]-ladderanol,[3] [5]-ladderanoic[4] acid as well as their unnatural analogues in an effort to unravel their biosynthetic hypothesis. In addition, our recent work on the enantioselective synthesis of an unnatural benzo-analogue of [3]-ladderanol through the application of our newly developed alkoxy-directed dienamine catalysis[5] will also be discussed.



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Bio-Sketch

Ramaswamy Murugavel
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Short Bio

Ramaswamy Murugavel received Ph.D. from IISc and carried out postdoctoral work at the University of Göttingen before joining IIT Bombay, where he is currently a J C Bose National Fellow and an Institute Chair Professor. He is also the Professor-in-charge of the IIT Bombay Institution of Eminence Project as well as the Head of the newly formed IITB Centre of Excellence in Critical Minerals, Metals, and Materials. He is a fellow of the Indian Academy of Sciences, the Indian National Science Academy, and the Royal Society of Chemistry. He has been conferred with J. C. Bose National Fellowship, Swarnajayanti Fellowship, Alexander von Humboldt Fellowship, DAE-SRC Outstanding Investigator Award, DFG Mercator Professorship, CNR Rao National Prize in Chemical Sciences, SC Bhattacharya Award for Excellence in Research in Basic Sciences, SASTRA-CNR Rao Award DAE Young Scientist Award, CRSI Silver Medal, MRSI Medal, and J. C. Ghosh Medal. His research is published in the form of more than 260 original articles.

Keynote Lecture (KNL-2)

Metal Phosphate Molecules and Materials for Energy Transition

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Reaction of phosphoric acid mono- and diesters with a divalent transition metal ion can produce molecular clusters, 1-D polymers, 2-D grids, or 3-D frameworks. Particularly interesting among this series of structural types are the 1-D polymers that are built from thermally labile di-tert-butyl phosphate. These polymers with an inorganic backbone and organic sidechains readily and cleanly decompose at temperatures close to 200 ^{o}C. The nanomaterials produced from such precursors have been studied extensively as both electro- and photocatalysts in OER, HER, and overall water splitting reactions.

The monoaryl phosphate, on the other hand, combines with Co^{2+} or Zn^{2+} in a donor solvent (L) leading to the isolation of tetranuclear metal phosphates $[(R)PO_3M(L)]_4$ (R = alkyl/aryl or alkoxy/aryloxy), whose inorganic core resembles the zeolitic D4R secondary building units (SBUs). In recent times, we have unravelled that it is possible to isolate even larger SBUs through small variations in the reaction conditions. Rationalization of building principles along with the use of this class of compounds for energy applications will be highlighted in this lecture.

For further representative publications, see: Murugavel & co-workers, *ACS Catalysis* **2023**, *13*, 8535; *Inorg. Chem*. **2022**, *61*, 6807 & **2020**, *59*, 13233; *J. Am. Chem. Soc.* **2017**, *139*, 39; *Chem. Commun*. **2019**, 55, 7994; *Angew Chem., Int. Ed.* **2019**, 16844; *Small*, **2020**, 1903334; *Chem. Mater.* **2024**, *36*, 6475; *ACS Mater. Lett.* **2024, 6,** 2126; *Chem. Asian. J***. 2025,** e202401177; *Dalton Trans.* **2026***, 55,* 1306; *J. Mater. Chem***.** *A.* **2026**, *14*, 1136; *Carbon*, **2026**, *249*, 121260.

Bio-Sketch

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Professional Experience

- Member of TPC for the Advanced Research Grant of ANRF (2025)
- Selection Panel Member for the Award of Ramanujan Fellowship of ANRF (2025)
- Guest Editor, *Communications Chemistry* (2025)
- International Advisory Board Member: *Angewandte Chemie Novit* (From 2025)
- Nomination Council Member of Infosys Prize (from 2024)
- Advisory Board Member: *Chemical Society Reviews* (From 2023)
- International Advisory Board Member: Chemistry Europe (from 2023)
- International Advisory Board Member: *Angewandte Chemie* (From 2021)
- Editorial Board Member: *ACS Applied Polymer Materials* (2021-2024)
- Early Career Editorial Board Member: *ACS Sust. Chem. & Engg* (2017-19)

Academic

2021-2025	Dean, Infrastructure and Planning, IISER-Thiruvananthapuram.
2020-date	Professor, School of Chemistry, IISER-Thiruvananthapuram.
2014-2019	Associate Professor, School of Chemistry, IISER-Thiruvananthapuram.
2009-2014	Assistant Professor, School of Chemistry, IISER-Thiruvananthapuram.
2008-2009	Senior Scientist, Institute of Life Sciences, Hyderabad.
2006-2008	AvH Postdoctoral Fellow, MPI for Molecular Physiology, Dortmund, Germany.
2004-2006	Research Officer, Department of Pharmacy & Pharmacology, University of Bath, UK.
2002-2004	JSPS Postdoctoral Fellow, Faculty of Engineering, Ehime University, Japan.
1997-2002	PhD, NCL Pune.

Awards & Honors

National Prize for Supramolecular Chemistry (2025); Society for Materials Chemistry (SMC) Silver Medal (2025); Elected Fellow of Indian National Science Academy (2025); JC Bose National Fellowship (from 2024); Silver Star Medal by Chirantan Rasayan Sanstha (2023); Excellence in Carbohydrate Research Award, by the Association of Carbohydrate Chemists & Technologists, India (2022); Rajib Goyal Prize by the Kurukshetra University, given annually to one chemist in India for outstanding research contributions (2021); Elected as Fellow of Indian Academy of Sciences (2020); Technology Innovation Award, Ministry of Chemicals & Fertilizers, Govt. of India (2020); Bhagyatara Award, by the Panajab University, given to one chemist annually for outstanding research contributions (2019); Author Profile appeared in the international journal, *Angewandte Chemie* (2018); Fellow of the Royal Society of Chemistry (2018): inducted as the Leader of the Field; MRSI Medal of Materials Research Society of India (2017); Bronze Medal of Chemical Research Society of India (2016); Young Scientist Award, Young Investigator's Meet (YIM)-Boston, MIT, USA (2015); Swarnajayanti Fellowship, Dept. of Science & Technology, Govt. of India (2013); Ramanujan Fellowship, Dept. of Science & Technology, Govt. of India (2010); Innocentive challenge award (20,000 $) for designing the shortest and economical route to tuberculosis-drug, PA-824 (InnoCentive 5636748, 2008)

Keynote Lecture (KNL-3)

Topochemistry for Solving Challenges in Polymer Synthesis

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Abstract

Topochemical reactions, the reaction between pre-organized reacting motifs in the crystal lattice, are attractive as they do not require solvents, catalysts and other special reaction conditions for the reaction and provide products in pure form. Also such reactions provide basic understanding about mechanistic and geometrical details about a reaction. We have employed thermal Topochemical Azide–Alkyne Cycloaddition (TAAC), Topochemical Ene-Azide Cycloaddition (TEAC) and Topochemical Diels-Alder Cycloaddition (TDAC) reactions to synthesize various biopolymer mimics. We have exploited hydrogen bonding for the self-assembly of monomers in solid to pre-organize the reacting motifs. Lattice controlled polymerization/oligomerization reaction of such self-assembled (pre-organized) monomers gave various biopolymer mimics. By applying this methodology, we have topochemically synthesized monodisperse glycopolymers, oligosaccharide mimics, DNA analogs and polypeptides.[1-9] In this talk, I will demonstrate the use of topochemical polymerization in the synthesis of ladder polymers, 2D polymers, stereocomplex, polymer-polymorphs etc.

References and Notes

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5. A. Lal, R. Rai, M. C. Madhusudhanan, K. M. Sureshan, *Angew. Chem. Int. Ed*., **2025**, *64,* e202503624
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Bio-Sketch

Prthasarathi Das
Professor and Dean (R&D)

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Ph: 9419227993
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Professional Experience

(2003-Till Date)

- Research Investigator (Chemistry-Lead) Aurigene Discovery Technologies Ltd. (Dr Reddy's Laboratories Ltd) Hyderabad, India
- Associate Director, Discovery Chemistry, Dr Reddy's Laboratories Ltd., Hyderabad, India.
- Principal Scientist, Department of Medicinal Chemistry, CSIR-Indian Institute of Integrative Medicine, Jammu, India.
- Associate Professor, Department of Chemistry & Chemical Biology, Indian Institute of Technology (ISM)Dhanbad, India.
- Professor, Department of Chemistry & Chemical Biology, Indian Institute of Technology (ISM) Dhanbad, India.

Academic

- Dean Research and Development, IIT (ISM) Dhanbad, Aug 2025-at present.
- Head of Department Chemistry and Chemical Biology IIT (ISM) Dhanbad, June 2021-July 2025.
- Head of Department, Department of Natural Product Chemistry, CSIR-IIM Jammu 2015-2017

Awards & Honours

- Research Council Member of CSIR-Indian Institute of Integrative Medicine, Jammu
- International Advisory Board Member of New Journal of Chemistry (NJC)
- Fellow of the Royal Society of Chemistry (FRSC)
- Council Member, Chemical Research Society of India (CRSI) (2020-2023)
- PEC Member, Technology Development Board (TDB), DST, Govt. India
- Chemical Research Society of India (CRSI) Bronze Medal 2019

Membership

- Indian Chemical Society (**ICS**), Kolkata, India
- American Chemical Society (**ACS**), USA
- Royal Society of Chemistry (**RSC**), UK
- Chemical Research Society of India (**CRSI**), Bangalore, India
- Indian Society of Chemists and Biologist (**ISCB**), Lucknow, India

Keynote Lecture (KNL-4)

Expanding Discovery Chemistry Toolbox: From Concept to Practice

Parthasarathi Das

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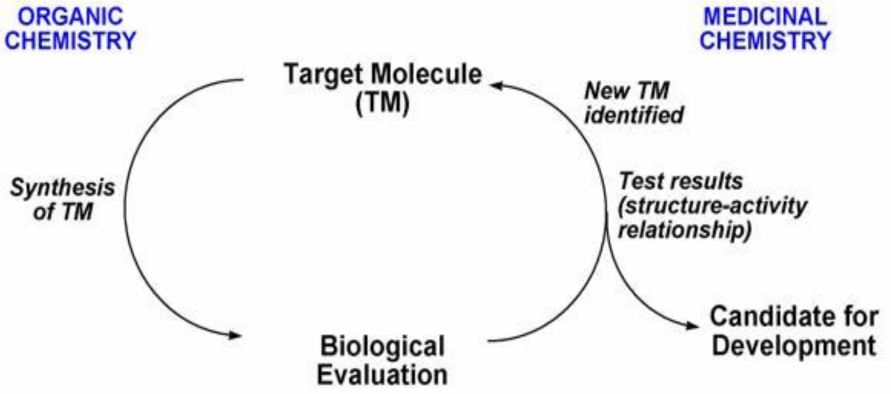
Abstract

The pharmaceutical and chemical industry remains solely reliant on synthetic methodology to prepare drugs or drug-like molecules for their discovery/process program. The expansion of synthetic methodology in recent years has greatly facilitated the preparation of heterocycles that would once have been considered an insurmountable synthetic challenge. In turn, the pharmaceutical industry, where large numbers of heterocycles are prepared and tested for their therapeutic use, became the principal end-users and beneficiaries of this enlarged toolkit. Designing and discussing transition-metal-promoted various synthetic tools for the synthesis of pharmaceutically important heterocycles and the generation of new chemotypes with translational potential will form the basis premise of my presentation[1-5].

Figure/Scheme:



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4. T. Roy, S. Jana, and **P. Das**, *J. Org. Chem.* **2025**, *90*, 9083-9097.
5. M. Deb, H. Singh, D. Manhas, U. Nandi, S. K. Guru, and **P. Das**, *RSC Med. Chem.* **2024**, *15*, 3097–3113.

Nitin T. Patil
Professor

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Professional Experience

- Professor (10/2023 - Present): Department of Chemistry, IISER-Bhopal, Bhopal
- Associate Professor (07/2017 - 10/2023): Department of Chemistry, IISER-Bhopal, Bhopal
- Senior Scientist (08/2013-06/2017): CSIR-NCL, Pune
- Senior Scientist (03/2011-08/2013): CSIR-IICT, Hyderabad
- QRS (09/2008-03/2011): CSIR-IICT, Hyderabad
- Research Fellow (01/2008-07/2008): The Scripps Research Institute, USA
- Research Fellow (06/2006-12/2007): Institute of Chemical and Engineering Sciences, Singapore
- Assistant Professor (04/2005-03/2006): Tohoku University, Japan
- JSPS Postdoctoral Fellow (11/2002-03/2005): Tohoku University, Japan
- Postdoctoral Fellow (03/2002-11/2002): University of Goettingen, Germany

Research Interests

Organic Synthesis, Metal Catalysis, Organocatalysis, Enantioselectivity, Organometallics, Total Synthesis etc.

Awards and Honours

- Recipient of the J. C. Bose Fellowship, CNR Rao National Prize for Chemical Sciences, SERB Distinguished Investigator Award, CRSI Bronze Medal, INSA Young Scientist Medal, Alkyl Amines – ICT Foundation Day Young Scientist Award, Avra Young Scientist Award etc.
- Fellow of the Indian National Science Academy (FNA), Fellow of The National Academy of Sciences (FNASc), Fellow of Indian Academy of Sciences (FASc), Fellow of Maharashtra Academy of Sciences (FMASc) and fellow of The Royal Society of Chemistry (FRSC).
- Editor of an Elsevier journal - Tetrahedron Letters (Year 2024 - present)

Keynote Lecture (KNL-5)

Enantioselective Gold Redox Catalysis

Nitin T. Patil

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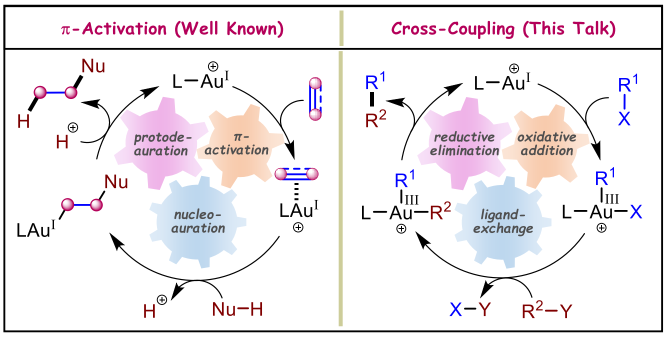
Abstract

Traditionally, gold complexes have been recognized as Lewis acid catalysts for the activation of C-C multiple bonds (Scheme, LHS). Over the years, there has been a considerable shift, and Au(I)/Au(III) redox catalysis is now recognized as an established technique for achieving cross-coupling reactivities (Scheme, RHS). The pioneering work by Zhang and Toste group revealed the role of external oxidants to overcome the high redox potential of Au(I)/Au(III) couple (E0 = +1.41 V) and to facilitate two-electron redox cycle in gold catalysis. Later, the Glorius group introduced the merged gold/photoredox strategy to circumvent the need for a stoichiometric oxidant in these processes. Recently, ethynylbenziodoxolones (EBXs) have also been used for accessing redox gold catalysis serving dual role as oxidant and alkyne surrogate.

All the above strategies were not amenable to the use of aryl halides, and thus their use in gold-catalyzed cross-coupling reactions remained forbidden. In recent years, ligand-enabled gold redox catalysis have emerged as a valuable tool, allowing for the use of aryl halides as cross-coupling partners. In this talk, I will present some of our recent work on enantioselective gold redox catalysis.



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Bio-Sketch

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Professional Experience

S. No.	Position & Organization	Period
1	Principle Scientist, Scientist-E, CSIR-CECRI	Nov-2024 to till date
2	Senior Scientist, CSIR-CECRI, Chennai Unit	Nov - 2021 to Nov 2024
3	Scientist, CSIR-CECRI, Chennai Unit	Nov - 2017 to Nov - 2021
4	DST-Inspire Faculty, CSIR-IICT, Hyderabad	Nov - 2016 to Nov - 2017
5	Post-doctoral Researcher, Tokyo Institute of Technology, Tokyo, Japan	June - 2015 to Oct - 2016
6	Project Assistant, CSIR-NCL, Pune	Jan - 2009 to April - 2012

Academic

S. No.	Degree	Institution	Year
1.	Ph.D.	Academy of Scientific and Industrial Research (AcSIR), New Delhi, India	2015
2	M.Sc.	Solapur University, Solapur, Maharashtra, India	2008
3	B.Sc.	Shivaji University, Kolhapur, Maharashtra, India	2004

Awards & Honors

- **National list**

1. Highest ECF Earning Scientist (2022-2023)
2. CSIR-SRF Fellowship (April 2012)
3. First Rank in M.Sc. (Physical Chemistry)

- **International list**

1. Kanagawa Academy of Science and Technology (KAST), Japan-Post doctoral Fellowship (June-2015)
2. Marie-Curie Fellowship Award (Feb-2017)
3. Life membership in the International Association for Hydrogen Energy (IAHE)
4. Outstanding Reviewers for the Journal of Materials Chemistry A in 2020, 2021

Technologies Process/Know-How Developed/ Transferred

1. Technology transfer of the LT-PEMFC system to M/s. KPIT, Pune (2021)
2. Advanced high-performance membrane electrode assemblies (2024)
3. Indigenous Pt-nanoparticles supported on carbon (Pt/C) as an alternate to the state-of-the-art Pt/C (2024)

Invited Lecture (IL-01)

Electrocatalyst and Electrolyte Engineering for Energy Applications

Vishal M Dhavale [a,*]

[a]CSIR-Central Electrochemical Research Institute (CSIR-CECRI), CSIR Madras Complex, Taramani,
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Abstract

The development of advanced PGM, non-PGM-based electrocatalysts for polymer electrolyte membrane fuel cells (PEMFCs) and the engineering of aqueous electrolytes for improved charge storability in aqueous Zn-ion battery (AZIBs) are crucial for the next-generation energy storage and conversion technologies. The multifaceted investigation into two distinct but related areas will be focused.

First, the beneficial role of a CoNi-alloy in facilitating the formation of N-doped bamboo knotted tube morphology via a tip-in growth mechanism. This unique structure establishes the CoNi-alloy as a highly promising Pt-free cathode electrocatalyst for anion exchange membrane fuel cells, addressing the need for efficient and cost-effective noble-metal alternatives.

Second, a revolutionary reverse dual-ion battery design that leverages a low-redox potential anode and a cation-deficient cathode to fundamentally alter ion de(insertion) chemistry within a $ZnCl_2$ water-in-salt electrolyte (WiSE). This innovative sequencing of ion-born chemistry represents a significant leap forward, showcasing groundbreaking potential for advancements in aqueous energy storage technology. Complementary to this, we provide molecular insights into the behaviour of methanol as an antisolvent in $ZnCl_2$ WiSE and experimentally evaluate its impact on the performance and efficiency of AZIBs. Understanding these interactions is vital for optimizing electrolyte formulations and enhancing battery longevity and capacity.

Lastly, the glimpse of design, development and demonstration (D3) of CECRI's PEMFC technologies in the stationary and automotive sectors will be discussed.

Keywords: PGM and Non-PGM Electrocatalyst, Dual-ion Battery, Antisolvents, PEMFC

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5. A Sethi, C Rajeev, A Kumar, SD Bhat, Vishal M Dhavale, Chemical Communications 61 (54), 9780-9801

Bio-Sketch

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Professional Experience

- 2026/01 - till date: Scientist 'G', Institute of Nano Science and Technology, Mohali, India.
- 2021/01 - 2025/12: Scientist 'F', Institute of Nano Science and Technology, Mohali, India.
- 2015/04 - 2020/12: Scientist 'E', Institute of Nano Science and Technology, Mohali, India.
- 2012/05 - 2015/03: Postdoc with Prof. JR Nitschke, University of Cambridge, UK. Research topic: Photophysics and host-guest properties of metal-organic cages.
- 2009/07 - 2012/04: Postdoc with Prof. FD Lewis, Northwestern University, Evanston, IL, USA.

Research topic

Self-assembly and electronic properties of chromophore functionalized oligonucleotides.
Photochemistry and Photophysics; Nanoscience; Nucleic acids; Supramolecular Chemistry

Invited Lecture (IL-02)

Broadening the Functional Scope of Imino(Boron) Compounds in Energy-Related Applications

Prakash P. Neelakandan

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Abstract

Schiff bases, characterized by the presence of the azomethine (-HC=N-) group, are easily synthesized via the condensation reaction between an aldehyde and an amine. These compounds are versatile chelating agents due to their multiple donor atoms, such as oxygen and nitrogen, which can coordinate with metal ions, anions, and biological molecules. Boron complexation significantly enhances the photophysical properties of Schiff bases, making them suitable for use as stimuli-responsive materials.[1] Boron complexes of Schiff bases are stabilized by the delocalization of electrons from the lone pairs on the heteroatoms into the vacant *p*-orbital of the boron center. This electron delocalization lowers the LUMO energy levels, resulting in red-shifted absorption and improved luminescence. The unique photophysical properties, ease of synthesis, and structural stability of boron complexes of Schiff bases make them ideal candidates for a variety of applications. We have successfully synthesized several Schiff bases and their boron complexes and studied their photophysical and optoelectronic properties. Notably, some of these compounds crystallized into single crystals exhibiting mechanical flexibility. The optical and mechanical features of these crystals were applied in sensing, catalysis, and energy harvesting.[2–5]

References and Notes

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Bio-Sketch

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Professional Experience

Postdoctoral fellow: 2015-2018 (Arieh Warshel, University of Southern California, LA)

Academic

Ph.D. 2010-2015 (R. B. Sunoj, IIT Bombay)
MSc and BSc: 2004-2009 (University of Delhi)

Awards & Honors

Rekha Rao Young Investigator Award (2021), The Ranganathan Family Endowment Fellow (2024), Priti Shankar Award in Teaching Excellence (2025), Thieme Chemistry Journal Awardee (2024)

Invited Lecture (IL-03)

Dirhodium Catalysts: From Mechanistic Aspects to Synthesis to Application

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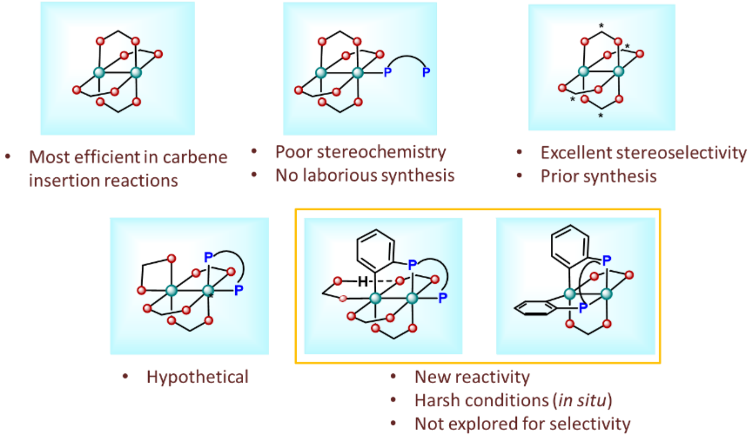
Abstract

Dirhodium tetracarboxylate catalysts enable a wide range of organic transformations with notable reactivity. However, their application in asymmetric synthesis remains challenging due to the rigid catalyst framework and the linear coordination geometry between substrates and ligands. Our mechanistic studies on carbene insertion reactions provide deeper insight into these structural constraints and their implications for catalyst design. Building on these findings, we explored ligand-driven modifications of dirhodium complexes. Using a combination of ^{31}P-NMR spectroscopy and DFT calculations, we show that light induces isomerization of the bisphosphine ligand from an axial to an equatorial position. These redesigned complexes exhibit enhanced reactivity in alkyne hydrosilylation under ambient conditions. Additionally, in another work, we demonstrate that the dirhodium catalyst dissociates into a monomeric species, which we successfully isolated and found to exhibit improved enantioselectivity in a carbonyl arylation reaction.

Figure: Dirhodium Catalysts and their Coordination Patterns with Bisphosphine Ligands



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Professional Experience

- **Ph.D. (2013)** under Prof. Martin Oestreich at Westfälische Wilhelms-Universität Münster (with research at TU Berlin); funded by the NRW stipend
- **Postdoctoral stints** at Université de Strasbourg (2013–14) under Prof. Françoise Colobert; KAIST, South Korea (2014–18) with Prof. Sukbok Chang; and KAUST, Saudi Arabia (2018–19) with Prof. Magnus Rueping

Academic

- **July 2023 – Present:** Associate Professor, Department of Chemistry, Indian Institute of Technology-Delhi, India.
- **March 2019 – July 2023:** Assistant Professor, Department of Chemistry, Indian Institute of Technology-Delhi, India.

Research Focus

Dr Hazra leads a research group specialising in metal-free catalysis, the activation of small molecules for the conversion of feedstock chemicals into value-added products, with an emphasis on gaining deep mechanistic insight and developing practical synthetic methodologies.

Awards & Honors

- Winning the **OPPI Young Scientist Award 2025**.
- **Thieme Chemistry Journals Award 2023**, one of 86 young chemists globally
- Awarded **Chirantan Rasayan Sanstha® (CRS) Bronze** Medal by Vidyasagar University.
- **Merck Young Scientist Award 2023** (Runner-up).
- Numerous research grants, including STARS, MHRD (**2023**), FIRP, IIT Delhi (**2022**), CSIR project (**2021**), and multiple SERB/DST (SRG, CRG etc) and IIT Delhi grants.

Academic Contributions

Dr. Hazra has made significant contributions to the field, with an impressive publication record that includes over 60 research works and more than 1327 Google Scholar citations (h-index: 20; i10-index: 32). His research has been featured in respected journals such as *Angewandte Chemie, Organic Letters, JACS Au, Green Chemistry, Chem Commun, Journal of organic Chemistry, Organic Chemistry Frontiers and Advanced Synthesis & Catalysis etc*. His work focuses on innovative metal-free transformations, including Friedel-Crafts alkylation, deoxygenative or reductive coupling, and C–H bond activation, which continue to advance the understanding of these important chemical processes.

Invited Lecture (IL-04)

Regioselective, Non-Directed C–H Functionalization of Small Molecules *via* Brønsted Acid Catalysis

Dr. Chinmoy Kumar Hazra*

*E-mail: chinmoy@chemistry.iitd.ac.in

Abstract

Rapid progress in the research of metal-free transformations has been observed in the past decades; however, there's still plenty of room to be solved. First part of my talk: This talk starts with the Brønsted acid-catalyzed Friedel-Crafts reaction to convert cheap chemicals into value-added products. Triarylmethanes are generally synthesised through metal-catalysed cross-coupling or Friedel–Crafts arylation, which involves harsh reaction conditions and pre-functionalized starting materials. Alternatively, we will use a cheap, commercially available Brønsted acid-catalytic system for the synthesis of unsymmetrical polyarylated alkanes from feedstock chemicals. Additionally, the method will be applicable to the late-stage functionalization of natural products, such as thymol, menthol, and eugenol. Second part: Reversing the conventional site-selectivity of C−H activation provides efficient retrosynthetic disconnections to otherwise unreactive bonds. In this part, I will focus on the Brønsted acid-catalyzed reaction that selectively performs meta-amination/arylation of anisidines with amines/arenes in a one-pot procedure. I will also focus on the scalability and functional group tolerance, including late-stage functionalization of pharmaceutical compounds and natural products. The control experiments and detailed computational analysis will be discussed to better understand the mechanism and the origin of meta-selectivity. Also, the synthesis of challenging drugs will be highlighted. Some ongoing projects will be discussed if time permits. The large-scale synthesis of pharmaceutically active ingredients using a metal-free protocol will be briefly discussed. Third part: Some ongoing projects will be discussed if time permits. Moreover, the large-scale synthesis of pharmaceutically active ingredients (APIs) via a metal-free protocol will be briefly discussed.

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[1] Singh, S.; Kumar, A.; Nebhani, L.; Hazra, C. K.* *JACS Au*. **2023**, *3*, 3400–3411.; [2] Taneja, N.; Sharma, P.; Yadav, N.; Musib, D.; Hazra, C. K.* *Org. Lett.* **2023**, *25*, 6029–6034.; [3] Yadav, N.; Taneja, N.; Musib, D.; Hazra, C. K.* *Angew. Chem. Int. Ed*. **2023**, *62*, e202301166. [4] Yadav, N.; Mahato, R.; Pal, S.; Dey, M.; Hazra, C. K.* *Org. Lett.* **2025**, *27*, 6566−6570.

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Professional Experience:

- **2013-2015**: Postdoc: Chubu University, Mentor: Prof. Hisashi Yamamoto
- **2016**: Alexander von Humboldt fellow: Westfälische Wilhelms-Universität Münster, Mentor: Prof. Frank Glorius
- **2016-2021**: Assistant Professor, Indian Institute of Science Education and Research Kolkata
- **2021-2025**: Associate Professor, Indian Institute of Science Education and Research Kolkata
- **2025**-: Professor, Indian Institute of Science Education and Research Kolkata

Academic:

- **200**7: B.Sc. University of Calcutta (Chemistry Hons.)
- **2009**: M.Sc. Indian Institute of Technology Kanpur (Chemistry)
- **2012**: PhD Ludwig Maximillan Universität Munich, Supervisor: Prof. Herbert Mayr

Awards & Honors:

- **2024**: Associate of the West Bengal Academy of Science & Technology (WAST)
- **2021**: Merck Young Scientist Award (runner-up) in Chemical Science
- **2021**: "2021 Young Investigator Award ", Sponsored by Molecules
- **2021**: INSA Medal for Young Scientists
- **2021**: Associate of the Indian Academy of Sciences (IASc)
- **2020**: NASI-Young Scientist Platinum Jubilee Award (2020) in Chemical Sciences
- **2019**: Thieme Journal Award
- **2016**: INSPIRE Faculty Award, DST

Invited Lecture (IL-05)

Expanding the Toolbox of Catalysis: From Light-Driven Dearomatization to Remote C–H Functionalization to Polymer Upcycling

Biplab Maji

Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata
E-mail: bm@iiserkol.ac.in*

Abstract

The development of new catalytic strategies that enable molecular complexity, precise bond functionalization, and sustainable chemical transformations is central to modern synthesis. This talk describes our efforts to expand the toolbox of catalysis through light-driven dearomatization, remote C–H functionalization, and polymer upcycling.

The conversion of planar aromatics into sp³-rich three-dimensional architectures, has emerged as an important design principle in medicinal chemistry. Dearomative cycloaddition reactions provide a direct route to such frameworks but are challenged by aromatic stability and selectivity issues. We report a visible-light-induced triplet–triplet energy-transfer catalytic platform that enables meta- and para-dearomative cycloaddition of naphthalene derivatives with tethered alkenes and vinyl benzenes. Mechanistic studies supported by computational and photophysical analyses elucidate the underlying energy-transfer process. The method exhibits broad scope, functional-group tolerance, scalability, and compatibility with late-stage functionalization.

We further address the challenge of regio- and enantioselective remote C–H functionalization using native directing groups. Through catalyst engineering, a chiral iridium system based on a 2,2′-bipyridine ligand analogue enables enantioselective meta-C(sp^2)–H borylation of diarylacetic acid–derived amides.

Finally, I will briefly highlight how catalytic concepts can be extended toward polymer upcycling, demonstrating how advances in catalysis can bridge molecular synthesis and sustainability. Collectively, these studies underscore how innovative catalytic strategies can unlock new reactivity paradigms across small-molecule synthesis and materials chemistry.

References and Notes:

4. J. Ma, S. Chen, P. Bellotti, R. Guo, F. Schäfer, A. Heusler, X. Zhang, C. Daniliuc, M. K. Brown, K. N. Houk, F. Glorius, *Science*, **2021**, *371*, 1338.
5. P. Rai, K. Maji, S. K. Jana, **B. Maji**, *Chem. Sci.*, **2022**, *13*, 12503.
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8. P. Rai, S. Naik, K. Gupta, K. Maji, G. Jindal, **B. Maji**, *Nat. Commun.* **2025***, 16*, 2991.
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10. A. Jati, D. Dam, T. T. Khan, **B. Maji**, *Angew. Chem. Int. Ed.* **2025**, *64*, e202510788.
11. S. Das Adhikari, S. K. Jana, **B. Maji,** *Angew. Chem. Int. Ed.* **2025***, 64, e202513145.*

Invited Lecture (IL-06)

Spintronics and Chirality: Spin Selective Electron Transport through Chiral Molecules

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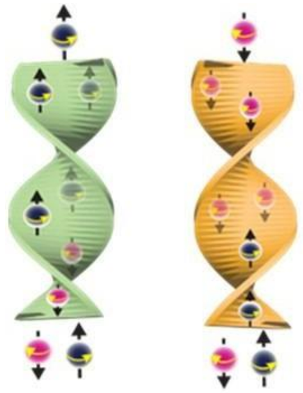
Abstract

Recent experiments have demonstrated that the electron transfer through chiral molecules depends on the electron spin orientation. This phenomenon has been termed the chiral-induced spin selectivity (CISS) effect,[1] and it provides a challenge to theory and promise for organic/inorganic molecule-based spintronic devices. Recently an efficient method to organic spintronic based on CISS effect has been suggested. In the CISS effect, the chirality of the molecular system itself acts as a spin-filter, thus avoiding the use of magnets for spin injection. Techniques for measuring spin- selective electron transport through molecules and some examples of recent experiments will be discussed.[2-5] By studying spin-dependent electron transport through various supramolecular structures, and inorganic chiral molecules, we can able to describe the possible application of the CISS effect for developing new kinds of memory devices. Such memory would be based on spintronics, the use of the electrons' spin, rather than charge. Furthermore, the CISS effect is a multidisciplinary phenomenon with implications in chemistry, physics and biology; therefore, this field has many-fold directions and will open new avenues for scientific and technological exploration.

Figure/Scheme:



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Bio-Sketch

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Professional Experience

1. Since 2009 – Haute École d’Ingénierie et d’Architecture Fribourg, Full Professor of Organic Chemistry & Process Chemistry
2. 2004–2009 – Zürcher Hochschule für Angewandte Wissenschaften, Professor of Organic Chemistry
3. 1999–2004 – CarboGen Laboratories AG, Scientific Director Process R&D; Senior Process Research Chemist
4. 1996–1997 – Sandoz Pharm. Corp., East Hanover, NJ, Post-Doctoral Fellow, Oncology
5. 1988–1989 – Ciba-Geigy AG, Basel, Research Chemist

Academic

1. 1993–1996 – ETH Zürich, Ph.D. in Chemistry with Prof. Dr. D. Seebach
2. 1989–1992 – ETH Zürich, Diploma in Chemistry
3. 1985–1988 – Höhere Technische Lehranstalt Winterthur, Diploma as Chemist HTL
4. 1982–1985 – ETH Zürich, Apprenticeship as Laboratory Assistant

Awards & Honors

1. Sandmeyer Award 2015 of the Swiss Chemical Society (CHIMIA 2016, 70, 502-511)
2. ETH Zurich Silver Medal 1992 for Diploma Thesis
3. Max Lüthi Award 1988 of the Swiss Chemical Society for the best diploma

Membership

1. Member of the Swiss Chemical Society (SCS), the Schweizerische Gesellschaft der Verfahrens- und ChemieingenieurInnen (SGVC), the American Chemical Society (ACS), and the Gesellschaft Deutscher Chemiker (GDCh)
2. Member of the executive committee of the Division of Industrial & Applied Chemistry (DIAC) of the Swiss Chemical Society
3. Head of the SATW topical platform “Chemistry”

Invited Lecture (IL-07)

Single-Atom Palladium Catalysts for Sonogashira Coupling: Bridging Green Metrics, Ligand Design, & Scale-Up

Roger Marti,[a]* Dario Poier,[a]

[a] Institute of Chemical Technology, Haute école d'Ingénierie et d'Architecture Fribourg, HES-SO University of Applied Sciences and Arts Western Switzerland, Boulevard de Pérolles 80, 1700 Fribourg, Switzerland

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Abstract

Catalysis is a cornerstone of the chemical industry's transition toward sustainability. Single-atom catalysis (SAC), dispersing individual metal atoms on solid supports, combines homogeneous selectivity with heterogeneous robustness. These novel catalysts boost activity and enable greener, more efficient transformations, as shown by recent advances in Pd-SAC catalyzed cross-coupling reactions.

We investigated various Pd single-atom catalysts for Sonogashira cross coupling reactions by optimizing reaction conditions (solvent, base, Cu co-catalyst). We further explored substrate scope and assessed stability and efficiency of the Pd-SAC. Scale-up and catalyst recycling were demonstrated for a key intermediate of the anticancer drug Erlotinib.

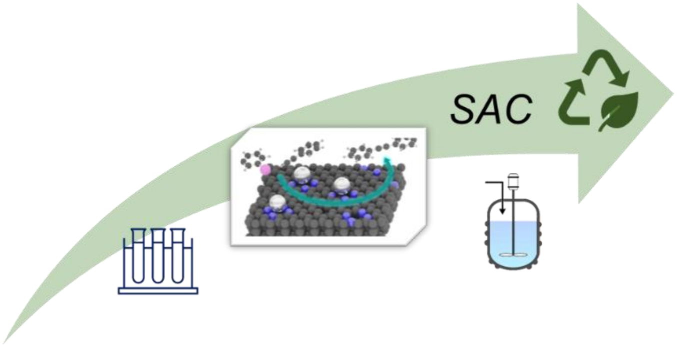

Figure: SAC for sustainable organic synthesis

This presentation details an interdisciplinary approach encompassing environmental assessment, mechanistic studies, reaction and ligand design, and scale-up trials of Pd single-atom catalysts for Sonogashira cross-coupling reactions.

References

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2. Poier, D. et al.; *ACS Sustainable Chem. Eng.* **2023**, *11,* 16935-16945.
3. Poier, D. et al.; *ACS Nano* **2025**, *19*, 1424−1432.

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Professional Experience

- Associate Professor, Institute for Catalysis, Hokkaido University, Japan, Apr. 2024 – Present
- Assistant Professor, Institute of Material Science, Faculty of Pure and Applied Science, University of Tsukuba, Japan, Apr. 2018 – Mar. 2024
- Specially Appointed Researcher, Department of Chemistry, Graduate School of Science, Kyoto University, Japan, Apr. 2017 – Mar. 2018
- Specially Appointed Researcher, Department of Chemistry, Graduate School of Science, Osaka University, Japan, Feb. 2015 – Mar. 2017
- Specially Appointed Researcher, Institute of Industrial Science, The University of Tokyo, Japan, Apr. 2014 – Jan. 2015
- JSPS Research Fellow (DC1), Department of Applied Physics, Graduate School of Engineering, The University of Tokyo, Japan, Apr. 2011 – Mar. 2014

Academic

- Ph.D. in Applied Physics, Graduate School of Engineering, The University of Tokyo, Japan, Apr. 2009 – Mar. 2014
- B.E. in Applied Physics, Faculty of Engineering, The University of Tokyo, Japan, Apr. 2005 – Mar. 2009

Awards & Honors

- Special Jury Prize & NEDO Award
- Platinum-Free Fuel Cell Catalysts Supporting Disaster Resilience and a Hydrogen Society, NoMaps2025 (STARTUP HOKKAIDO), Sep. 2025
- Paper Award
- Experimental Verification of Mixed-Potential-Driven Catalysis, The Japan Society of Vacuum and Surface Science, Jul. 2025
- Young Scientist Award
- The Physical Society of Japan (Studies on flow and controlling factor of energies in surface reactions), Oct. 2022
- Young Faculty Award, University of Tsukuba, Jul. 2021

Membership

- American Vacuum Society (AVS), The Japan Society of Vacuum and Surface Science
- The Catalysis Society of Japan, The Physical Society of Japan

Invited Lecture (IL-08)

Hybrid thermochemical–electrochemical catalysis enabled by mixed potentials: design of green CO_2 conversion reactions

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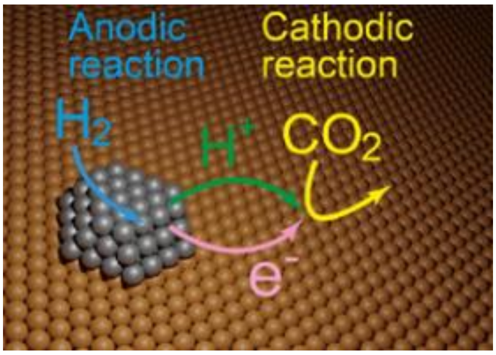
Abstract

Catalytic reactions are traditionally classified into thermochemical reactions driven by heat and electrochemical reactions driven by external electrical bias. In this study, we introduce mixed-potential-driven catalysis as a hybrid reaction concept that bridges these two domains, enabling chemical transformations without external power input. In mixed-potential systems, anodic and cathodic electrochemical reactions proceed simultaneously on coupled catalytic sites, forming a self-generated electric field that acts as the driving force for the overall reaction.

We experimentally verified the existence of mixed-potential-driven catalysis using spatially separated and electrically connected catalyst pairs. Spontaneous short-circuit currents were directly observed, demonstrating the formation of mixed potentials under reaction conditions. Kinetic analysis based on Butler–Volmer-type models revealed that reaction rates and selectivity are governed by overpotential partitioning between the coupled half-reactions, providing a quantitative design principle for this hybrid reaction field.

As a key application toward sustainable chemistry, we applied this concept to CO_2 conversion using Cu-based catalysts for CO_2 reduction coupled with H_2 oxidation on Pd-based catalysts. Under relatively mild conditions (373 K, 40 atm), the system produced not only CO and methanol but also C_2 products such as ethanol, which are rarely obtained in conventional thermocatalytic systems. The product selectivity was found to correlate with the initial mixed potential and the oxidation state of Cu, demonstrating that CO_2 conversion can be designed through electrochemical parameters even in the absence of an external bias.

These results establish mixed-potential-driven catalysis as a third catalytic framework, distinct from thermocatalysis and electrocatalysis, and provide a new strategy for green and sustainable chemical conversion. The concept offers a platform for designing self-powered reaction fields applicable to CO_2 utilization and other complex catalytic reactions.



Schematic of CO_2 conversion by using mixed potential

References and Notes

1. M. Yan, J. Nakamra, K. Takeyasu et al., Communications Chemistry 7:69 (2024).
2. M. Yan, K. Takeyasu et al., ChemCatChem, e202400322 (2024).
3. M. Yan, K. Takeyasu, J. Nakamura et al., Adv. Sci. e05994 (2025).
4. K. Takeyasu, J. Nakamura et al., e-JSSNT 21, 164 (2022).

Bio-Sketch

Sandeep Kaur
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Professional Experience

- 2023-present **Professor**, Department of Chemistry, University of Delhi
- 2020-2023 **Associate Professor**, Department of Chemistry, University of Delhi
- 2010-2020 **Assistant Professor**, Department of Chemistry, University of Delhi
- 2018-2019 **Researcher**, Leibniz Institute for Catalysis, Rostock
- 2009-2010 **Postdoctoral Fellow**, Dept of Photochemistry and Molecular Science, Uppsala University
- 2007-2008 **Postdoctoral Fellow**, Department of Chemistry, Stanford University

Academic

- 2012-2016 **Max-Planck India Fellow**, MPI for Dynamics of Complex Technical Systems
- 2011 & 2012 **Visiting Scientist**, Uppsala University, Sweden
- 2005 **Visiting Researcher**, Stuttgart University
- 2002-2007 **PhD**, Department of Chemistry, IIT Bombay
- 2000-2002 **M.Sc**, Burdwan University, West Bengal
- 1997-2000 **B.Sc**, Hooghly Mohsin College, Burdwan University

Selected Publications

1. Ritu; Kaur-Ghumaan, S., *J. Molecular Structure,* **2025**, *1353*, 144398.
2. Agarwal, T.; Joshi, M.; Ritu; Stein, M.; Kaur-Ghumaan, S., *Organometallics,* **2024**, *43*(24), 3096-3105.
3. Agarwal, T.; Kaur-Ghumaan, S., *Eur. J. Inorg. Chem*., **2023**, *26*(11), e202200623.

Awards & Honors

- Research Publication Award from IoE, University of Delhi
- Indo-US Research fellowship from DST, India and Indo-US Science & Technology Forum (IUSSTF) (declined)
- Wenner-Gren Fellowship, Sweden
- Participant, 56th Nobel Laureate Meeting in Chemistry, Lindau

Membership

- Alumni, Global Young Academy (2019-2025) &
- Organization for Women in Science for the Developing World (OWSD)
- Materials Research Society of India, Bangalore & Catalysis Society of India, Chennai
- Indian Council of Chemists, Agra & Chemical Research Society of India (CRSI)
- Indian Science Congress Association, Kolkata & Indian Chemical Society, Kolkata

Invited Lecture (IL-09)

Hydrogen Evolving Mono-nuclear Complexes with Carefully Positioned Ligands

Sandeep Kaur-Ghumaan[a*]

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Abstract

Enormous efforts have been made by the scientific community in the development of bio-mimetic/bio-inspired hydrogen-evolving complexes as catalysts for an alternative hydrogen energy carrier and renewable energy sources. Inspired by nature, till date several di-nuclear systems have been reported as hydrogen evolution reaction (HER) catalysts using a combination of a wide variety of ligands and conditions but relatively few well-defined mono-nuclear systems are known. Furthermore, though mononuclear nickel complexes-especially DuBois-type systems with proton-relaying phosphine-amine ligands and cobalt complexes, including cobaloximes and polypyridyl derivatives, have been widely studied for photochemical and electrochemical H_2 production, challenges remain in improving catalyst stability, integrating molecular catalysts into practical devices and achieving high activity at low driving force. Mono-nuclear complexes continue to play an important role in developing efficient and sustainable catalysts for hydrogen production. Ligand design plays a central role, with proton relays and redox-active frameworks significantly reducing overpotentials and accelerating key steps. Herein, transition metal-based mononuclear systems with carefully positioned ligands reported by our group will be discussed. The discussion will include synthesis, characterization and electrocatalytic applications of such catalysts integrating both experimental and theoretical methodologies. Theoretical DFT calculations enable a detailed picture of catalytic pathways, assign redox transitions and structural changes.

References and Notes

1. Hussein, F. A.; Joshi, M.; Kaur-Ghumaan, S.; Stein, M.; *ChemCtaChem*, **2024**, *16*, e202400450.
2. Kaim, V.; Joshi, M.; Stein, M.; Kaur-Ghumaan, S.; *Int. J. Hydr. Energ.,* **2023**, *48*, 30718-30731.
3. Kaim, V.; Joshi, M.; Stein, M.; Kaur-Ghumaan, S.; *Front. Chem.,* **2022**, *00*, 1-13.
4. Kaim, V.; Kaur-Ghumaan, S.; *New J. Chem.,* **2021**, *20272-20279*.
5. Agarwal, T.; Kaur-Ghumaan, S.; *Inorg. Chim. Acta*, **2020**, *504*, 119442.
6. Kaur-Ghumaan, S.; Hasche, P.; Spannenberg, A.; Beweries, T.; *Dalton Trans.*, **2019**, *48*, 16322-16329.

Bio-Sketch

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Professional Experience

Academic

M.Sc., & M.Tech. IIT, Delhi; D. Phil. from the University of Oxford; PDF from the University of Nottingham and the University of Oxford; Lecturer (retained) at University of Oxford.

Awards & Honors

- Associate Editor, ACS Macromolecules
- The first Most Creative Research Award Polybenzoxazine Community,
- CRSI Bronze award,
- APA Young Scientist Award,
- Amongst 75 WOMEN IN CHEMISTRY in “SHE IS”
- Chemistry–An Asian Journal Lecture Award.
- BIRAC-SRISTI GYTI (Gandhian Young Technological Innovation) award,
- Distinguished alumna award,
- Research Excellence Award@ Shiv Nadar University,
- DST Young Scientist Award

Membership

Vice President, SPSI; Council Member of the CRSI; Chief Executive Member of Sustainability Forum, APA; and member of ACS, RSC, and ICS

Invited Lecture (IL-10)

Circular Thermosets: Transforming Concepts into Sustainable Solutions

Prashansa Gupta, Bhavika Bhatia and **Bimlesh Lochab**

[a] Department of Chemistry, School of Natural Sciences,
Shiv Nadar (Institution of Eminence) University, INDIA

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Abstract

The escalating depletion of fossil fuel reserves, coupled with the growing burden of waste accumulation, underscores the urgent need for sustainable polymeric materials. Polybenzoxazines, a class of thermally curable thermosetting resins, exhibit superior thermal, mechanical, and chemical properties compared to conventional phenolic resins. Importantly, their synthesis aligns with green chemistry principles—utilizing bio-renewable feedstocks, operating under solvent-free conditions, and generating minimal toxic byproducts. Our research group leverages the molecular design versatility of polybenzoxazines to enable copolymerization with diverse comonomers, including elemental sulfur [1–4]. This structural adaptability also facilitates stimulus-responsive depolymerization, paving the way for closed-loop recycling strategies. These attributes render polybenzoxazines highly suitable for advanced applications such as re/debondable adhesives, antibacterial coatings, water purification membranes, battery cathodes, and self-healing materials.

Figure/Scheme: Caption

References and Notes

1. P. Gupta; S. Rastogi; B. Bhatia; S. Yadav; B. Lochab; A*CS Sustainable Chem. Eng.,* **2025,** *13*, 10, 4055–4067.
2. B. Bhatia, P. Gupta, C. Len, B. Lochab, *Macromolecules*, **2025**, *58*, 10725–10737.
3. S. Sahu, B. Lochab, *ACS Sustainable Chem. Eng.*, **2024,** *12*, 7126.
4. V. Duhan; S. Yadav; C. Len; B. Lochab, *Green Chem.*, **2024**, *26*, 483.

Bio-Sketch

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Group Homepage: https://www.aklab-iitp.com/

Career profile

- Associate Professor, IIT Patna: **5th Dec. 2019**
- Assistant Professor, IIT Patna**: 2014-4th Dec. 2019**
- Research Investigator-Bristol M.R. C., Bangalore**: 2012- 2013**
- Postdoctoral Fellow-University of Konstanz, Germany**: 2010-2012**
- Postdoctoral Fellow -City University of New York, USA: **2008-2009**
- Ph. D. IIT Kanpur, India: **2008**
- M. Sc. Delhi University: **2002**

Honours and awards

- Dr. H C Srivastava Memorial Award-**2024** by ACCT(I)
- Editorial Board Member: ***Journal of Carbohydrate Chemistry from 2024***
- CRSI-Bronze Medal Award **2023**
- Council Member, CRSI-**2023-2026**
- Executive Member ACCTI- **2023-2026**
- Life-member-**CRSI, India**
- Life-member-**ISCB, India**
- Life-member- **ACCT, India**

AK research group is primarily involved in the design and development of cost and atom-economical strategies for the synthesis of important functional organic molecules utilizing the chemistry of primary amides and imidates. The 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 is also involved in the glycodiversification aspects of carbohydrate chemistry.

Representative Publications

1. *Chem.Commun.* **2022**, *58,11304*
2. *J. Org. Chem.* **2021**, *86, 9744*
3. *Org. Letter,* **2020**, *22, 5, 1908*
4. *Org. Letter,* **2020**, *22,4,1605*
5. *J. Org. Chem.* **2019**, *84, 589*
6. *Org.Lett.* **2018**, *20, 4964*
7. *Org.Lett.* **2018**,*20,4964*
8. *Chem.Commun.* **2018**, *57, 7207*
9. *J. Org. Chem.* **2018**, *83, 12247*
10. *J. Org. Chem.* **2016**, *81, 661*

Invited Lecture (IL-11)

From Simple to Complex: Synthesis of Key Heterocyclic Compounds

Amit Kumar*

Department of Chemistry
Indian Institute of Technology Patna, Bihar, India

(E-mail: amitkt@iitp.ac.in)

Abstract

Functionalized heterocyclic molecules play a crucial role in natural products and biologically active compounds, making them highly significant in organic synthesis. The introduction of desired functional groups while adhering to principles of sustainable chemistry such as cost-effectiveness and atom economy is in high demand. Direct functionalization of inert C-H (sp^2/sp^3) bonds offers an efficient and attractive approach for converting these unreactive sites into valuable chemical entities.[1] However, achieving regio- and chemo-selectivity remains a major challenge in such transformations.

To address these issues, the concept of directing groups (DGs) has been introduced, enabling selective functionalization. Over the past decade, various DGs have been developed to facilitate regioselective C-H activation. However, these approaches often require pre-installation and subsequent removal of DGs, adding extra steps and thereby reducing the overall atom and step economy. Despite the widespread occurrence of primary amides and imidates in organic molecules, their use as directing groups has been largely overlooked due to their low reactivity, making them challenging yet intriguing synthons. Given their abundance and synthetic potential, we aimed to explore primary amides and imidates as effective directing groups for the synthesis of high-value organic derivatives.[2] This presentation will discuss the scope and limitations of this approach through selected examples.

References

1. Lyons, T.W.; Sanford, M. S. *Chem. Rev*. **2010**, *110*, 1147.
2. (a) Y. Kumar, Y. Jaiswal and A. Kumar *Org.Lett.*_**2018**,*20*,4964. (b) **Kumar, Y.,** Jaiswal, Y., Kumar, A. *J. Org. Chem.* **2016**, *81*, 12247. **(c) Kumar, Y.,** Shaw, M., Thakur, R., Kumar A. *J. Org. Chem.* **2016**, *81*, 6617

Short Invited Lecture (SIL-1)

ULTRA-STABLE LIQUID CRYSTAL-IN-WATER EMULSIONS AS OPTICAL BIOSENSORS

Abhijit Dan

Department of Applied Chemistry, Maulana Abul Kalam Azad University of Technology,
Simhat, Haringhata, Nadia - 741249, West Bengal

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Abstract

Micrometer-sized droplets of thermotropic liquid crystals (LCs) dispersed in aqueous media (i.e., LC-in-water emulsions) respond sensitively to the presence of a variety of different analytes that trigger changes in the configurations of the LC within the droplets.[1] Hereby, the analyte triggers a transition within LC droplets from a so-called ‘bipolar-to-radial’ configuration, visible from changes in the optical appearance of the droplets when observed using polarized optical microscopy. However, this method is not optimal as the basis of an analytical method for accurate quantification of a range of aqueous analytes for several reasons such as lack of stability of bare LC droplets, difficulty to image the droplets because of their translational and rotational mobility, and their conformational change resulting from sedimentation. In this study, we sought to develop a new strategy that involves formation of microgels decorated LC droplets by emulsifying a two- phase system wherein the organic (oil) phase is a low molecular weight LC, nematic 4-cyano-4'-pentylbiphenyl (5CB) while the aqueous phase is a dispersion of microgel particles in water. This approach provides an excellent stability to the LC emulsion droplets, the stability of which can be further tuned by incorporating charged moieties in the microgels as well as by preparing core-shell microgels. Microgels coating eliminates the droplet−surface interactions caused by sedimentation and change droplet mobility in aqueous medium, thus this approach facilitates the characterization of LC droplets using polarized light microscopy. In order to study the ability to respond to the presence of added analytes after microgels coating, we characterize the LC droplets by observing the optical appearances upon the addition of sodium dodecyl sulfate (SDS) as a model analyte. The LC-in-water emulsions can be broken at temperature slightly above the volume phase transition temperature (VPTT) of the microgels that results macroscopic phase separation, thereby leading to recycling of the emulsifiers.[2] The combination of excellent emulsion stability and breaking on-demand, the responsivity of the droplets and the reusability of the emulsifier offers a complete and versatile toolbox for sustainable application of biological sensing.

References and Notes

1. Lin, I.-H.; Miller, D. S.; Bertics, P. J.; Murphy, C. J.; De Pablo, J. J.; Abbott,
2. N. L. ***Science*** 2011, 332, 1297–1300.
3. **Dan, A.**; Agnihotri, P.; Brugnoni, M.; Siemes, E.; Woll, D.; Crassous, J. J.; Richtering, W. **Chem. Comm.** 2019, 55, 7255—7258.

Bio-Sketch

Dr. M. Shiva Prasad
Associate Professor

Department of Chemistry
Room No: 404, Block-C, Department of Chemistry, Faculty of Science, North Campus, University Delhi, Delhi-110007.

Email: sprasadm@chemistry.du.ac.in and shivacutn@gmail.com
Ph: 9491634764
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Professional Experience

- Associate Professor – Since July, 2025
- Assistant Professor- Selection grade -July 2022-June 2025
- Assistant Professor- Senior grade- July 2017- June 2022
- Assistant Professor- Stage I- June 2013-June 2017

Academic:

- Ph. D. Chemistry- University of Hyderabad
- MSc. Chemistry-Osmania University

Awards & Honors

- National Overseas Postdoctoral Fellowship-Govt. of India -2016
- CSIR- Senior Research Fellowship -2010-2013
- CSIR-Junior Research Fellowship- 2008-2010

Membership:

- Member of The Royal Society of Chemistry (MRSC)-since 2019
- Life Member-Chemical Research Society of India-CRSI-since 2014
- Member of American Chemical Society (2019-2021)
- Member of Board of Studies- CUTN (2016-2019 & 2022-2025)

Short Invited Lecture (SIL-2)

Aminocatalytic Asymmetric Remote Functionalization to Access Biologically Potential Scaffolds

Madavi S. Prasad[a,*] M. Sivaprakash,[b] and S. Bharani[b]

[a]Department of Chemistry, University of Delhi, Delhi-110007.
[b]Department of Chemistry, Central University of Tamil Nadu, Thiruvarur-610005.

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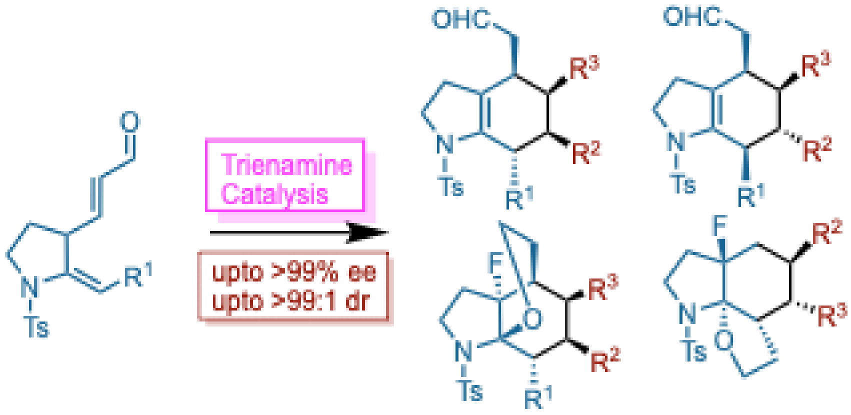
Abstract

This talk describes the preparation and reactivity of a newly designed pyrrolidine-linked dienal employed in a remote [4+2] annulation *via* an in situ generated trienamine species. The transformation afforded the targeted products in moderate to high yields with outstanding stereocontrol. Notably, the work reveals, for the first time, an unusual inversion of a distant stereocenter under trienamine activation. The versatility of the method was further highlighted by a two-pot, three-step protocol enabling access to spirocyclic, bridged, and tricyclic perhydroindole frameworks reminiscent of natural product motifs.

Scheme: Aminocatalytic Asymmetric Remote Functionalization



References and Notes

1. Prasad, M. S.; Sivaprakash, M.; Bharani, S.; *Chem. Asian J.* **2023**, *18*, e202300419.
2. Prasad, M. S.; Sivaprakash, M.; Bharani, S.; *Org. Biomol. Chem.*, **2023**, *21*, 945 - 949.
3. Prasad, M. S.; Jha, A. K.; Bharani, S.; *Adv. Synth. Catal.*, **2024**, *366*, 2014 - 2019.

Flash Talk (FT-01)

Metal-Organic Frameworks (MOFs) for CO_2 Capture from Air

Arijit Mallick

School of Environmental Sciences, Jawaharlal Nehru University, New Delhi, India
E-mail: arijitmallick@jnu.ac.in

Abstract

Global warming and associated climate changes are one of the biggest challenges faced by humanity in recent times. An increase in atmospheric CO_2 concentration over the last century, mainly owing to industrial and vehicular CO_2 emissions, is directly related to global warming. Metal-organic frameworks (MOFs) have shown the potential to qualify as disruptive materials for applications pertaining to gas storage, separation technologies, and pollutant control. However, such materials, mostly fabricated in powder form, are brittle and can easily break into fine powders when conventional shaping/forming strategies are implemented. Therefore, the development of advanced CO_2 capture physical adsorbents in powdered form is a key step. Nevertheless, their transformation into particulates is a process of paramount importance for their deployment and implementation in real-world applications. Herein, I will present a facile and quick shaping process of one of the best solid-state materials, KAUST-7 (NbOFFIVE-1-Ni), for CO_2 capture at trace concentrations. The CO_2 adsorption by KAUST-7 is mainly driven by strong intermolecular interaction and is purely physical- based adsorption. Purposely, KAUST-7 powder was transformed into shaped bodies using select polymers as binders, and their associated CO2 capture properties were thoroughly evaluated before and after shaping. Then, these materials were incorporated into a prototype device for a CO_2 capture application.

Keywords: Carbon Capture; Metal-Organic Frameworks; Adsorption; Scaleup Synthesis.

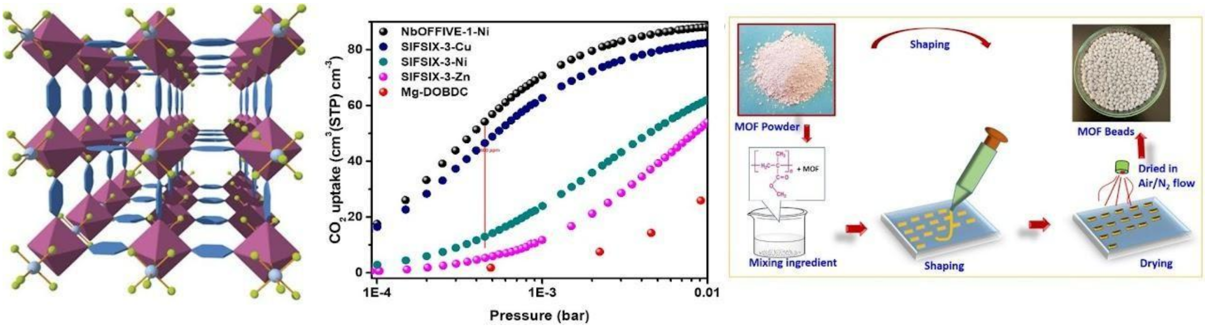


Figure: Represents the KAUST-7 MOF structure and its CO_2 adsorption behaviour at low pressure. The materials were synthesized in bulk and shaped into beads using polymer binders**.**

References

- A. Mallick, *et. al. Ind. Eng. Chem. Res.*, 2018, **57**, 16897–16902
- P. M. Bhatt, M. Eddaoudi *et al. JACS*, 2016, **138**, 9301−9307.

Bio-Sketch

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Professional Experience

Since 09.2023 Assistant Professor; **Indian Institute of Technology Gandhinagar**, India
09.2021 – 09.2023 Postdoc in the group of **Prof. Theodor Agapie**, Department of Chemistry and Chemical Engineering, **California Institute of Technology** (Caltech), USA
04.2018 – 06.2021 Postdoc in the group of **Prof. Jun Okuda**, Institute of Inorganic Chemistry, **RWTH Aachen University**, Germany

Academic

- 2011 – 2017 Dr. rer. nat., (*Summa cum laude*), University of Bonn, Germany.
- 2009 – 2011 M.Sc. (Chemistry), Indian Institute of Technology Kanpur, India.
- 2006 – 2009 B.Sc. (Chemistry), Ramakrishna Mission Residential College Narendrapur, Calcutta University, India.

Awards & Honors:

- Manik Chandra Award, **2009**: For securing the top position (77.75%) in B.Sc. from Ramakrishna Mission Residential College Narendrapur, Kolkata, India.
- Awarded ACC (The Associated Cement Companies) fellowship, **2010** (IITK).
- Selected as one of the top 45 finalists among *ca*. 450 candidates for the **2016** Reaxys PhD Prize and attended the Reaxys PhD Prize Symposium in London, United Kingdom.
- Awarded Springer Theses Prize **2019** for outstanding PhD research.

Flash Talk (FT-02)

Transforming Dinitrogen into Trisilylamine via Homogeneous Titanium Catalysis

Priyabrata Ghana,[a,*] Jun Okuda[b,*]

[a]Department of Chemistry, Indian Institute of Technology Gandhinagar, India

[b]RWTH Aachen, Germany

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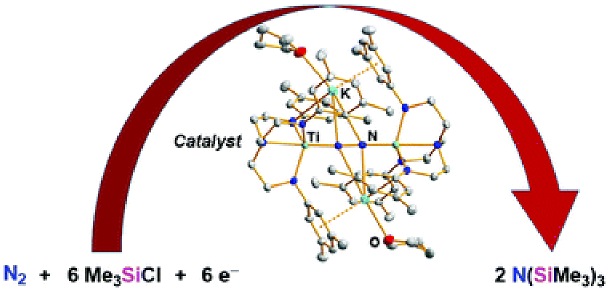
Abstract

The fixation of dinitrogen (N_2) to ammonia (NH_3) is one of the most important chemical reactions from both an industrial and a biological perspective. However, having one of the strongest chemical bonds known (BDE = 944 kJ mol^{-1}), and with a high ionization potential, large HOMO–LUMO gap, and no permanent dipole, there are major kinetic and thermodynamic barriers to activating N_2. Continuous research over the last several decades has shown that tailor-made mid- to late-transition metal complexes can fix N_2 to NH_3 or higher value products under both homogeneous and heterogeneous conditions.[1,2] In this talk, I will show that early transition metals, such as titanium, can also join the league and catalytically fix dinitrogen to trisilylamine under ambient conditions (Scheme 1).



Scheme 1. First catalytic fixation of dinitrogen to trisilylamine by a homogeneous titanium catalyst

References and Notes

- Y. Tanabe, Y. Nishibayashi, *Chem. Soc. Rev.* **2021**, *50*, 5201
- S. Kim, F. Loose, P. J. Chirik, *Chem. Rev*. **2020**, *120*, 5637.

Bio-Sketch

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Professional Experience

- Current position: Assistant Professor at Krea University, Sri City, AP, India [since September, 2025]
- Post Doc research at Chungbuk National University South Korea under Professor Isaac Choi [March-August, 2025]
- Post Doc research at Shiv Nadar IoE Deemed to be University under Professor Subhabrata Sen [March, 2024 to February 2025]
- Pre-graduation experience- Served Glenmark Pharmaceuticals Ltd in Sales and Marketing Division [March, 2008 – August, 2017]

Academic

- B.Pharmacy from Institute of Pharmacy, Jalpaiguri, WB [2007]
- MBA from IISWBM Kolkata [2014]
- M.Tech. in Pharmaceutical Technology from University of Calcutta [2018]
- Ph.D. in Organic Chemistry from Shiv Nadar IoE Deemed to be University [2024]

Awards & Honors

- G-LAMP Postdoctoral Fellowship (South Korea)
- RSC Horizon Perkin Prize 2025 in Organic Chemistry received as a team from Prof. Subhabrata Sen's group
- 'Star Performer' for 5 different years while working in Glenmark Pharmaceuticals Ltd

Membership

- Life time membership of CRSI, India

Flash Talk (FT-03)

Electrooxidative Divergent Halocyclizations of Ambident Amides

Minki Jeon,[a,#] **Debajit Maiti,[b,#]** Geon Kang[a], Jinwoo Kim,[c,*] and Isaac Choi[a,*]
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[b]School of Interwoven Arts and Sciences (SIAS), Krea University, Sri City 517 646, India
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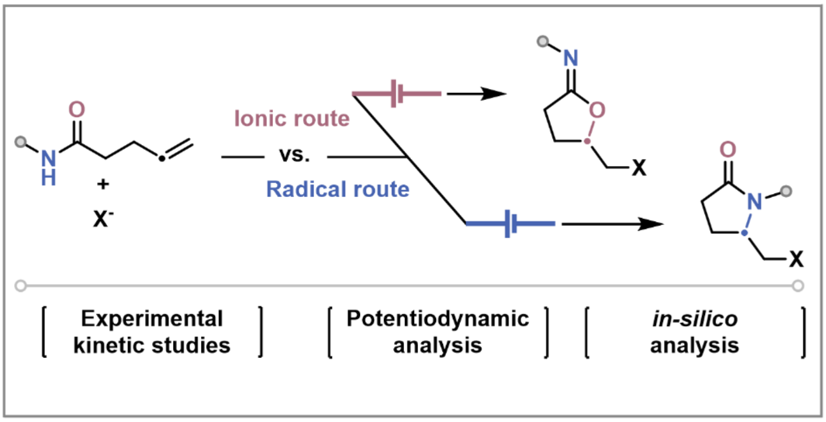
[#]contributed equally

Abstract

In this article, we reported a divergent electrochemical halocyclization of ambident amides that enables selective construction of either C–O or C–N bonds from a common substrate platform. The observed chemoselectivity is dictated by anodic oxidation conditions. Under chloride-mediated oxidation, haliranium ion formation promotes intramolecular C–O bond formation, whereas basic conditions favor amidyl radical generation, directing selective C–N bond formation. Detailed mechanistic insights were obtained through a combination of cyclic voltammetry, kinetic experiments, and in silico studies, which collectively elucidate the distinct reaction pathways. This electrooxidative strategy exhibits broad functional group tolerance and underscores the versatility of electrochemistry as a sustainable and precise tool for controlling ambident reactivity in halocyclization reactions.



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Flash Talk (FT-04)

Transforming The Chemically Impossible Into Scalable Reality Via Electrochemistry.

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Abstract

Eliteck is building a next-generation organic electrosynthesis platform with the vision of transforming chemically impossible, extremely difficult, or multistep reactions into scalable, single-step electrochemical processes. At the core of this effort lies Eliteck's deep expertise in electrochemistry combined with its indigenous capability to design, manufacture, and customize complete electrochemical systems, enabling seamless translation from laboratory discovery to industrial application.

Eliteck has successfully developed and manufactured proprietary electrochemical instrumentation, including the Orgel electrochemical reactor platform and electrochemical flow systems, specifically engineered for complex organic transformations. In parallel, Eliteck designs and fabricates a wide range of cost-effective, indigenous electrodes (carbon, graphite, nickel, copper, magnesium, and hybrid systems), allowing precise control over interfacial chemistry while maintaining scalability and economic viability. This vertically integrated approach—spanning electrochemical theory, reactor engineering, electrode development, and manufacturing—provides a unique foundation for systematic innovation in organic electrosynthesis.

Through industrial collaboration, multiple challenging reaction classes have already been accessed, including **C–C coupling, C–O coupling, and selective C–H functionalization**, enabling late-stage functionalization of complex, drug-like molecules. These electrochemical strategies convert conventionally multistep synthetic routes into direct, electron-driven transformations, offering improved selectivity, sustainability, and process simplicity.

By uniting deep electrochemical understanding with indigenous manufacturing of reactors, flow platforms, and low-cost electrode technologies, Eliteck establishes a powerful, scalable ecosystem for discovering new reactivity and translating organic electrochemistry into practical, industrially deployable solutions.

Orgel for Electro-Organic Synthesis

Poster Presentation (P-01)

Photochemical Dehydrogenation *via* Intermolecular Hydrogen Atom Transfer Reaction

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Abstract

Photochemical transformation of organic frameworks has experienced substantial advancement in recent decades, with photoredox catalysis emerging as a powerful strategy for sustainable organic synthesis. However, applications of precious metal-based photocatalytic transformations are limited due to high cost, limited recyclability, and scarcity of transition metals in nature.[1] Herein, we report a metal-free, visible-light-driven dehydrogenation of 6,5-bicyclic heterocycles via an intermolecular hydrogen atom transfer reaction without requiring transition metals, external oxidants, or harsh reaction conditions. The newly developed dehydrogenation process afforded α,β-unsaturated arylketones from sulfur and oxygen-containing bicyclic heterocycles with excellent functional group tolerance toward both electron-withdrawing and electron-donating groups (EWGs/EDGs).

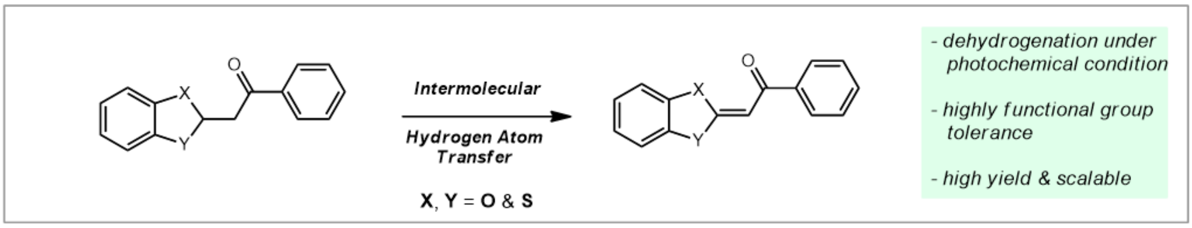

Figure: Synthesis of α,β-unsaturated arylketones via photoinduced HAT.

A detailed mechanistic study established the radical nature of this dehydrogenation process, and an EPR study confirmed the involvement of an oxygen-centred radical intermediate in the intramolecular hydrogen atom transfer process. These findings establish the photochemical dehydrogenation process as a viable alternative to transition metal catalysed protocols systems for selective dehydrogenation reactions under environmentally benign conditions.

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Poster Presentation (P-02)

Multiscale Computational and Experimental Insights into Mutation-Induced Structural Instability and Cofactor Binding Perturbations in Valosin-Containing Protein

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Abstract

Valosin-containing protein (VCP) is a multifunctional AAA+ ATPase that plays a central role in cellular proteostasis, including ER-associated degradation (ERAD), ubiquitin-dependent protein turnover, and organelle quality control [1]. Disease-associated mutations within its N-terminal domain, notably the Arg95Gly (R95G) substitution, have been linked to multisystem proteinopathies such as inclusion body myopathy with Paget's disease and frontotemporal dementia (IBMPFD) and amyotrophic lateral sclerosis (ALS). However, the structural & molecular basis by which these mutations impair VCP function remains unexplored [2]. Here, we utilized an integrated computational and experimental approach to delineate the structural and dynamic effects of the R95G mutation on the VCP N-domain and its interaction with the gp78 cofactor peptide. Our workflow combined AlphaFold3-based structural modeling, protein-peptide docking, and multiscale molecular dynamics simulations employing both all-atom and coarse-grained MD simulations. Detailed analyses of physicochemical properties, intermolecular contacts, and free-energy landscapes revealed that the mutant VCP-N-gp78 complex exhibits reduced structural stability, decreased compactness, and weakened intermolecular interactions compared to the wild-type complex. Consistently, MM/PBSA-based binding free energy analyses indicated a substantial loss in binding free energy and altered residue-specific energetic contributions upon mutation. These computational findings were further experimentally validated through recombinant expression and purification of the VCP N-domain, followed by biophysical characterization and isothermal titration calorimetry, which confirmed diminished binding affinity and reduced stability of the mutant complex. Collectively, this study provides mechanistic insight into mutation-driven VCP dysfunction and establishes a robust framework for exploring therapeutic interventions in VCP-associated proteinopathies.

Keywords: Valosin-containing protein, AlphaFold3, protein-peptide docking, molecular dynamics simulations, therapeutic interventions

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Poster Presentation (P-03)

Oxidative copper-catalyzed synthesis of β-amino ketones from allyl alcohols and anilines

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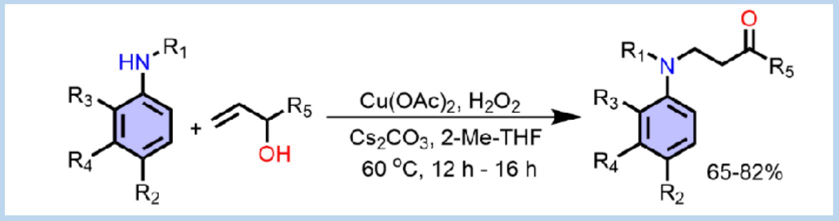
Abstract

In this article, we have reported the oxidative copper-catalyzed synthesis of β-amino ketones from allyl alcohols and anilines. The β-aminoketones are pivotal in heterocyclic synthesis, serving as essential scaffolds for diverse synthetic molecules.[1] They are widely available in natural products, drugs, and bioactive molecules.[2-4] We have developed a copper-catalyzed method for synthesizing β-amino ketones using allyl alcohols and substituted anilines in 2-methyl-THF at 60 °C.This reaction employs hydrogen peroxide ($H2O2$) as the oxidant and cesium carbonate as the base. The cost- effectiveness and high yield (65–82%) make this process a valuable alternative to the Pd-catalyzed coupling reaction of allylic alcohols with substituted anilines or substituted N-alkyl anilines.[5]



Scheme 1: Cu-catalyzed synthesis of β-amino carbonyl compounds.

Keywords: Amination, β-aminoketones, heterocyclic synthesis, indolines, and quinolines.

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Poster Presentation (P-04)

Substrate-Free Growth of N-Doped Bamboo Tube Morphology on CoNi Alloy Nanoparticles as an Electrocatalyst for Anion Exchange Membrane Fuel Cells

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Abstract

In the realm of fuel cell technology, the quest for durable and economical electrocatalysts persists as a critical endeavour. Herein, we introduce a durable electrocatalyst boasting a resilient knotted bamboo tube-like morphology, termed "*tip-in* grown", achieved through a single-step synergistic catalytic pyrolysis method. The innovative approach involves the diffusion of carbon atoms on CoNi-alloy nanoparticles, resulting in nitrogen-doped bamboo-like carbon tubes encapsulating CoNi-alloy nanoparticles (CoNi@NC-T). Notably, this architecture not only fosters ample cavities for facilitating induced current generation but also induces a non-uniform distribution of local charges due to nitrogen doping, thereby enhancing conduction and polarization. Furthermore, the confinement of CoNi-alloy within the carbon tubes effectively prevents nanoparticle aggregation and shields the alloy from corrosion, ensuring stable performance even in harsh chemical environments. Our study delves into the intricate interplay of temperature, thermal polymerization of dicyandiamide and catalytic role of CoNi-alloy nanoparticles in shaping the derived morphology, elucidated through meticulous replication of reaction conditions via thermo-gravimetric analysis (TG-DSC). Remarkably, CoNi@NC-T exhibits activity on par with state-of-art Pt/C catalyst for oxygen reduction reaction (ORR) and demonstrates unparalleled robustness, evidenced by a minimal shift in $E_{1/2}$ value after an extensive 30,000 potential cycling. Corroborating its durability, FE-SEM analysis confirms the retention of the bamboo-tube morphology on post-cycling. CoNi@NC-T as a cathode catalyst in an anion exchange membrane fuel cell (AEMFC).

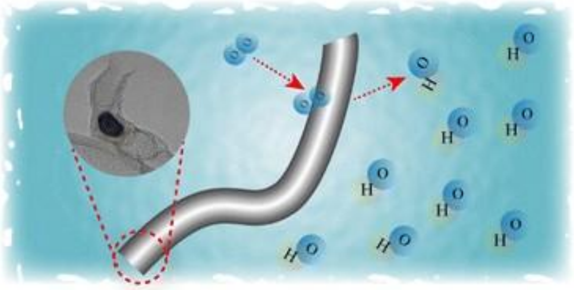

Figure: The beneficial role of the CoNi-alloy for the formation of N-doped bamboo knotted tube morphology *via* the tip-in growth mechanism as a Pt-free cathode electrocatalyst for anion exchange membrane fuel cells.

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Poster Presentation (P-05)

Metal-Free Direct Esterification of Aldehydes Using Hydroxylamine-*O*-Sulfonic Acid

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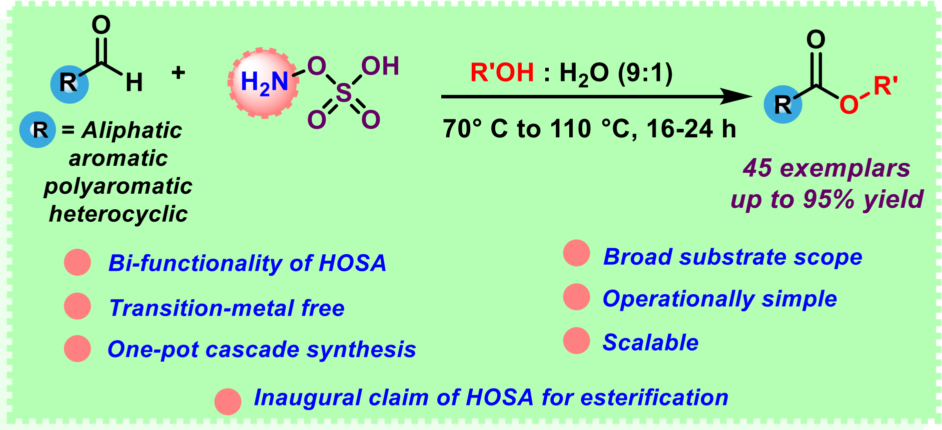
Abstract

Esters are ubiquitous structural motifs and key intermediates in the synthesis of diverse pharmaceuticals and bioactive molecules. Conventional esterification strategies often rely on expensive metal catalysts and harsh reaction conditions, which limit efficiency and substrate compatibility. Despite significant advances, the selective synthesis of substituted esters remains a persistent challenge.

In this work, we introduce a metal-free esterification protocol in which bi-functional hydroxylamine-*O*-sulfonic acid (HOSA) reacts with aldehydes in the presence of alcohols to furnish the corresponding alkyl alkanoates and benzoates. The transformation proceeds through the insitu formation of nitrile and imidate intermediates, enabling smooth conversion under mild conditions. The method is applicable to aliphatic, aromatic, polycyclic, and heteroaromatic aldehydes, delivering the corresponding esters in good to excellent yields while exhibiting broad functional-group tolerance. Further mechanistic insights and full experimental details will be presented during the conference.



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Poster Presentation (P-06)

Organocatalytic Regioselective Construction of C_2- and C_3-Symmetric Aryl Ketones via 6-π Electrocyclization

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Abstract

Highly symmetrical arenes featuring distinct motifs are gaining significant attention for their promising applications in medicine, nonlinear optical materials, supramolecular assemblies, and functional polymer materials. One of the most noteworthy approaches for constructing aromatic rings is alkyne trimerisation, an atom-economic method that offers flexibility based on specific requirements. While numerous methodologies utilising metal catalysts have been developed to create benzene rings, achieving precise control over regioselectivity remains a challenge due to the potential formation of isomers.

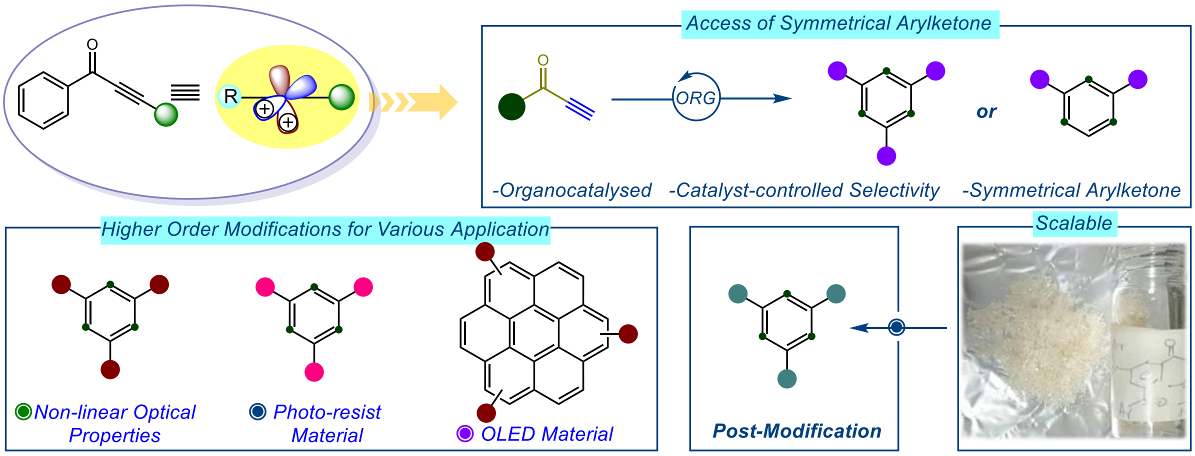

Figure: Organocatalysed synthesis of symmetrical polyaromatic hydrocarbons.

Herein, we are going to showcase the creation of highly symmetrical benzene rings through organocatalyzed 6π-electrocyclization. By strategically modifying the catalyst and fine-tuning the positioning of functional groups, we have successfully directed the reaction to exclusively yield the desirable 1,3-symmetrical product. This has enabled us to synthesise 1,3-symmetrical polyaromatic compounds, an endeavour that has historically presented significant challenges. Moreover, we have advanced these to produce macrocyclic symmetrical molecules that hold immense promise for applications in material chemistry, & OLED. These molecules are not only structurally sophisticated but are also recognised for their remarkable second-order nonlinear optical properties, which are currently under investigation.

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Poster Presentation (P-07)

BIFUNCTIONAL AROMATIC AMINE-CATALYZED AZA-FRIEDEL-CRAFTS/OXA-6Π CASCADE: SYNTHESIS OF 2,2-DISUBSTITUTED CHROMENES

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Abstract

In this article, we have reported Bifunctional Aromatic Amine-Catalyzed Aza-Friedel-Crafts/Oxa-6π Cascade: Synthesis of 2,2-Disubstituted Chromenes. The details will be presented during the conference. 2,2-disubstituted chromene holds significance in medicinal and materials chemistry due to its presence in bioactive molecules and optoelectronic.[1,2] Most existing approaches rely on transition-metal catalysis.[3,4] We developed a mild, organocatalytic method using phenols and *β*, *β*-disubstituted enals as the coupling partner to construct the frameworks. A bifunctional 2-amino pyridine catalyst enables cooperative activation, affording broad substrate compatibility, including variously substituted phenols and enals, yielding diverse chromene derivatives.[5]

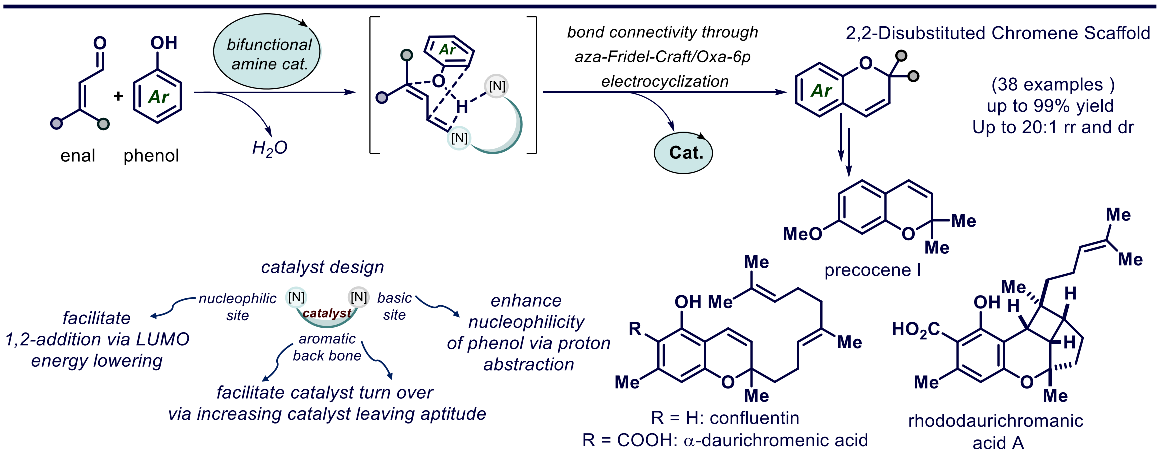

Figure 1: Organocatalytic one step approach to 2, 2-disubstituted chromene

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Poster Presentation (P-08)

Surface-Engineered Pt–Ni Catalysts for Improved Electrochemical Performance in Direct Ammonia Fuel cells

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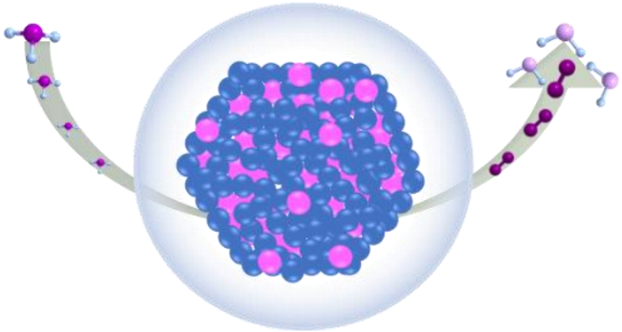
Abstract



Pt–Ni Alloy Catalyst Architecture for Enhanced Ammonia Oxidation

We have reported a nanostructured platinum-nickel (Pt–Ni) alloy catalyst as an efficient electrocatalyst for ammonia oxidation, addressing key challenges in direct ammonia fuel cells (DAFCs). The global transition toward clean and sustainable energy technologies has intensified interest in carbon-free energy carriers, where ammonia has emerged as a promising alternative to hydrogen due to its high volumetric energy density, high hydrogen content, and ease of storage and transportation. Despite these advantages, the practical implementation of DAFCs is severely hindered by the sluggish kinetics of the ammonia oxidation reaction (AOR). This limitation arises mainly from the formation and accumulation of strongly adsorbed reaction intermediates on the catalyst surface, leading to catalyst poisoning and reduced activity. In our work, we have developed a flower-like Pt–Ni alloy nanostructure with an enhanced surface-to-volume ratio and a well-ordered atomic arrangement. This tailored architecture improves reactant accessibility, mitigates intermediate poisoning, and promotes efficient low-temperature ammonia oxidation. The detailed synthesis strategy, structural characterization, and electrochemical performance evaluation of the Pt–Ni catalyst will be presented during the conference.

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Poster Presentation (P-09)

Designing *p*-block Metal-based Single Atom Catalysts for the Oxygen Reduction Reaction

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Abstract

The oxygen reduction reaction (ORR) is a key electrochemical process that governs the efficiency of fuel cells and metal–air batteries; yet it remains kinetically sluggish and heavily reliant on precious metal catalysts. Recently, p-block element–based single-atom catalysts (SACs) have emerged as promising alternatives due to their maximum atom utilisation, tunable electronic structures, and distinctive p-orbital–dominated catalytic behaviour. In this work, we focus on the rational design of p-block single-atom catalysts for ORR, emphasising the role of isolated p-block atoms (such as Bi, Sb, Sn, In, & Al) anchored on suitable supports, particularly heteroatom-doped carbon matrices. The strong hybridisation between the p orbitals of the single-atom centres and oxygen-containing intermediates enables optimised adsorption energies, reduced reaction energy barriers, and favourable reaction pathways compared to conventional d-band transition-metal catalysts. Furthermore, the local coordination environment and electronic interaction between p-block atoms and supports are shown to critically influence ORR activity, selectivity, and durability. These abstract highlights recent advances in catalyst design strategies, structure–property relationships, and mechanistic insights for p-block SACs in ORR, guiding the development of cost-effective, high performance electrocatalysts for next-generation energy conversion technologies.

Poster Presentation (P-10)

Guest-Dependent Charge Transfer and Folding of NDI-Oligomers

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Abstract

Nature has demonstrated a remarkable strategy for efficient light harvesting and energy storage through photosynthesis, which sustains life on Earth. With the growing global energy demand, achieving a sustainable energy future has become increasingly challenging, driving the development of alternative approaches in which artificial photosynthesis has emerged as a promising solution. In natural light-harvesting systems, the precise organization of chromophores within a protein matrix enables extended orbital interactions that facilitate efficient charge separation; in contrast, artificial systems largely rely on non-covalent interactions.[1] A major challenge in constructing such complex systems lies in achieving well-defined long-range ordering of chromophores while simultaneously controlling aggregate size and arrangement.[2] Foldamer-based architectures offer a strategic platform to address these challenges, wherein a defined number of chromophores are covalently linked to form multilayer π-stacks reminiscent of β-sheets in proteins, thereby enabling properties unattainable in monomeric analogues. Among various chromophores, naphthalenediimide (NDI) has emerged as a promising candidate owing to its attractive electrochemical and photophysical properties.[3] Herein, we report a synthetic strategy for covalently linked, electroactive, and conformationally flexible NDI oligomers, specifically tetramers and pentamers with a defined number of NDI units.[4] These oligomers exhibit multielectron reduction behavior dependent on oligomer length, solvent-dependent folding, and polyaromatic guest-induced tunable charge-transfer absorption. Charge transfer in the folded state enables alternate cofacial stacking of donor-acceptor units, providing insights into the design of ordered π-stacked materials with diverse optoelectronic functions.

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Poster Presentation (P-11)

Rational Design of Tunable Pyrylium Derivatives for intracellular pH mapping

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Abstract

Structural modulation of pyrylium-based fluorophores offers a powerful means to precisely tune their electronic and photophysical characteristics. Here, we report a new class of asymmetric, one-sided-bridged pyrylium fluorophores that bridge the structural gap between fully open and locked architectures. This hybrid topology enables controlled tuning of donor's strength, conformational rigidity, and fluorescence tunability. Systematic variation of peripheral substituents from electron-withdrawing to electron-donating groups and heteroatom replacement **(O→NMe** and **S)** in pyrylium lead to synthesis of a diverse library of pyrylium, pyridinium and thiopyrilium analogues displaying broad emission shifts (blue to red) and distinct quantum yields. Notably, this unique synthetic route offers simple, and structural diversity with excellent yields. Partial bridging significantly tune optical phenomena by balancing molecular rigidity and flexibility. Among the library, the thiopyrilium derivative **SMM-OH** demonstrates ratiometric fluorescent probe at longer wavelength compared to its pyridinium and pyrylium derivatives. It exhibits interesting localization within lysosomes and nuclei. This unique behavior enables dynamic, organelle-specific imaging and real-time mapping of subcellular pH microenvironments. These findings establish new thiopyrilium scaffold as versatile fluorophore for next-generation bioimaging probes.

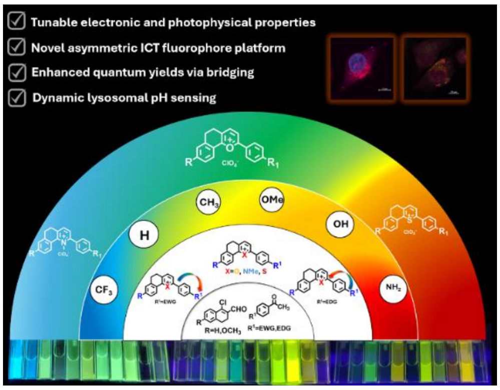

Fig: Representative figure illustrating the design and properties of the new fluorophore platform

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Poster Presentation (P-12)

Overcoming the deactivation mechanism in N-doped carbon catalysts in acidic electrolyte??

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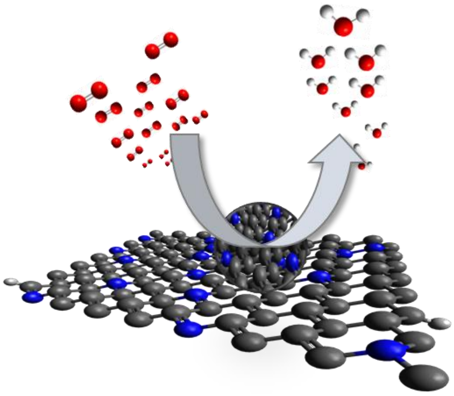
Abstract

Metal-free N-doped carbon (N–C) is highly active for alkaline oxygen reduction (ORR) but deactivates in acid due to pyridinic-N protonation and the energetically demanding *OOH reduction step. Here we engineer phosphorus in proximity to pyridinic-N to stabilise the active configuration, suppress protonation, and reprogram the ORR pathway.[1] The resulting catalyst, P, N–pC-7, is prepared by a double-calcination strategy and shows pH-universal activity with onset potentials of 0.87 V (pH 1) and 0.93 V (pH 13) vs RHE, approaching Pt/C benchmarks. Electrochemical analysis indicates ~99% selectivity for the $4e^-$ route. Further density functional theory reveals that carbon neighbours to P and adjacent C to pyri-N act as electron donors to populate O_2 π* orbitals, lowering the barrier for *O–O bond cleavage and enabling a dissociative pathway that bypasses *OOH as the rate-limiting intermediate while improving proton transport. A dual-atom motif further stabilises *OOH via bidentate coordination, narrows the free-energy gap between *OOH and *OH, and disrupts conventional scaling relations, collectively accelerating ORR kinetics in acid. In situ Raman spectroscopy corroborates the altered intermediate evolution under acidic operation.[2-3] This work establishes a design principle for acid-stable, metal-free carbon catalysts by coupling site protection with pathway control to deliver high ORR activity across a wide pH window.



Key Words: Electrocatalysis, metal-free catalyst, N-doped graphene, ORR mechanism.

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Poster Presentation (P-13)

Towards understanding gene regulation by SAM-II / SAM-V tandem riboswitch using fluorescence techniques

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Abstract

Riboswitches are short, gene-regulatory, non-coding nucleotide sequences located upstream of the coding regions in bacterial mRNA. They undergo conformational interconversions in response to the binding/unbinding of specific metabolites, leading to transcriptional or translational gene regulation. The gene being regulated typically encodes for a protein responsible for the homeostasis of the target metabolite, thus functioning in a feedback mechanism crucial for bacterial survival.[1] Therefore, molecular understanding of the metabolite binding and gene regulatory mechanisms of riboswitches is important for their applications as potential antibiotic drug targets. S-adenosyl methionine (SAM) is an important metabolite regulated by six different classes of riboswitches. Breaker and coworkers identified a tandem SAM-II/SAM-V riboswitch in which an upstream transcriptional 'SAM-II aptamer' and downstream translational 'SAM-V aptamer' regulates the same gene as RNA logic gate.[2] Towards understanding the molecular mechanisms of gene regulation by this tandem riboswitch, we first studied individual FRET-pair labelled SAM-II and SAM-V riboswitches using steady-state and single-molecule fluorescence techniques. Here, we primarily report the results from SAM-V riboswitch. We observe that the SAM-V riboswitch transitions from a low-FRET 'hairpin' structure to a high-FRET 'pseudoknot' structure upon binding to Mg^{2+}, a co-factor to several riboswitches, with Kd ~ 8 mM. Furthermore, while SAM binds to the riboswitch with Kd ~ 40 μM at physiologically relevant 2 mM Mg^{2+} concentration, it shows more an order of magnitude lower affinity in the absence of Mg^{2+}. These preliminary results suggest the binding of SAM to the SAM-V riboswitch in a Mg^{2+}-dependent conformational selection mechanism. We plan to validate this hypothesis as well study the folding-unfolding and ligand binding kinetics of SAM-II and SAM-V riboswitches, both individually and in tandem, using advanced single-molecule fluorescence studies.

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Poster Presentation (P-14)

Continuous-Flow Photochemistry for 1,4-Dioxane Remediation at Environmentally Relevant Concentrations

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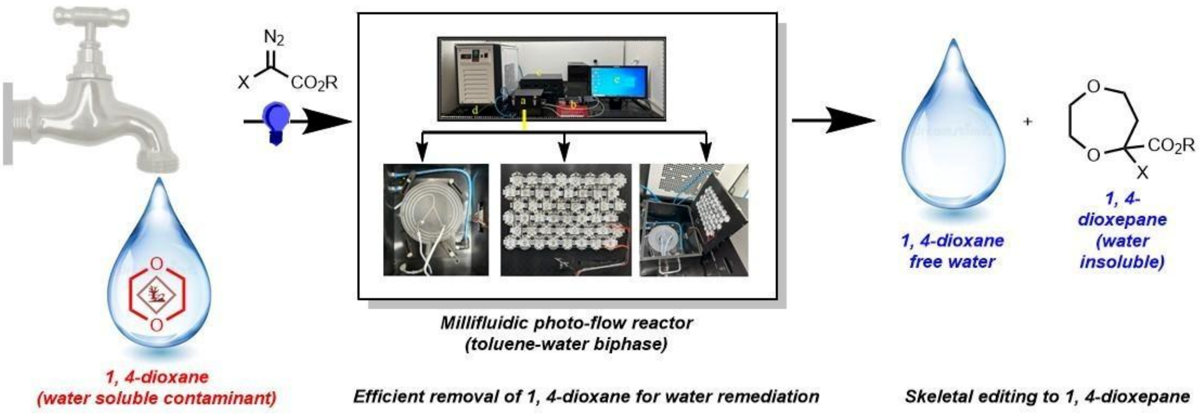
Graphical Abstract



Abstract

1,4-Dioxane, a probable human carcinogen and emerging groundwater contaminant, is highly resistant to conventional remediation methods. In our earlier work, we demonstrated a visible-light skeletal editing approach for its selective transformation, but only under unrealistically high aqueous loadings (~4.5 kg/L [51 M]). Here, we advance this concept to an oxidant-free continuous-flow photochemical platform that achieves efficient 1,4-dioxane remediation at environmentally relevant concentrations (~1 g/L [11.4 mM]). Using blue LED irradiation and aryl diazoacetates as carbene precursors, selective C–O bond insertion converts 1,4-dioxane into hydrophobic dioxepanes[1] that are readily separated from water. A biphasic segmented flow millifluidic reactor, optimised through Design of Experiments (DoE) and Generalised Linear Modelling (GLM) [2] ensured superior photon utilisation and interfacial mass transfer. Under optimised spiral geometries, the system achieved >93% conversion, with up to 95% removal efficiency at 1 g/L. This modular, energy-efficient strategy establishes a scalable and sustainable alternative to mineralisation-based approaches for 1,4-dioxane remediation.

Keywords

1,4-Dioxane, millifluidic photoreactor, skeletal editing, biphasic droplet flow, and water purification

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Poster Presentation (P-15)

Identifying the Rate-Determining Step in Oxygen Reduction Reaction on Nitrogen-Doped Carbon for Enhanced Catalyst Activity

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Abstract

Nitrogen-doped carbon catalysts are promising alternatives to Pt-based catalysts for fuel cell applications due to their metal-free nature and high durability. However, their insufficient catalytic activity for the oxygen reduction reaction (ORR) remains a critical challenge. To enable rational catalyst design, identifying the rate-determining step (RDS) is essential. Our previous work demonstrated that pyridinic nitrogen (pyri-N) at carbon edges forms the active sites, which exist as pyridinium (pyri-NH^+) under fuel cell operating conditions. We also found that the electrochemical reduction of pyri-NH^+ coupled with oxygen adsorption is a key elementary step [1]. (Table 1)

In this study, we identified the RDS through comprehensive kinetic analysis combining three approaches: acid-base equilibrium constant measurements, reaction order analysis using the rotating disk electrode, and ex-situ X-ray photoelectron spectroscopy (XPS) under applied potential. The pK_a of pyridinic nitrogen was determined to be 2. Near the onset potential, the Tafel slope was -125 mV/dec with oxygen and proton reaction orders of 1 and 0.4, respectively. Ex-situ XPS measurements showed the presence of pyri-NH^+ in the low current region, confirming that the coupled pyri-NH^+ reduction and oxygen adsorption step is indeed the RDS.

Based on these findings, we designed a novel nitrogen-doped carbon catalyst with a cage-like structure to increase hydrophobicity around the active sites. This design suppresses the hydration stabilization of pyridinium, thereby shifting its redox potential to more positive values. Our rational design approach successfully achieved a 0.2 V positive shift in the onset potential, demonstrating significant improvement in ORR activity.

Table 1: Reaction orders when each elementary step is rate-determining.
(Tafel slope = -120 mV/dec, pK_a of pyri-N = 2)

Elementary Step	O_2 reaction order	H^+ reaction order	Tafel slope (mV/dec, α=0.5)
1) $\text{pyri-N} + H^+ \rightleftarrows \text{pyri-NH}^+$	-	-	-
2) $\text{pyri-NH}^+ + O_2 + e^- \rightarrow O_{2,ads}\text{-pyri-NH}$	1	0.5	-120
3) $O_{2,ads}\text{-pyri-NH} + H^+ + e^- \rightarrow OOH_{ads}\text{-pyri-NH}$	0	1	-120
4) $OOH_{ads}\text{-pyri-NH} + H^+ + e^- \rightarrow O_{ads}\text{-pyri-NH} + H_2O$	0	1	-120
5) $O_{ads}\text{-pyri-NH} + H^+ + e^- \rightarrow OH_{ads}\text{-pyri-NH}$	0	1	-120
6) $OH_{ads}\text{-pyri-NH} \rightarrow H_2O + \text{pyri-N}$	0	0	-60

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Poster Presentation (P-16)

Ultrafast Synthesis of Conductive 2D Metal–Organic Frameworks

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Abstract

Metal–Organic Frameworks (MOFs) have recently attracted considerable attention as promising electrode materials for energy storage devices such as supercapacitors and batteries. Despite their potential, the widespread application of MOFs is limited by their intrinsically low electronic conductivity and complex synthetic routes. The poor conductivity of conventional carboxylate-based MOFs arises mainly from insufficient electronic conjugation within their frameworks. To overcome these limitations, current research efforts are increasingly directed toward the development of conjugated, electrically conductive MOFs that can fully exploit their high surface areas for efficient charge storage. However, the scalable and low-cost synthesis of such conductive MOFs remains a major challenge due to the complexity of their formation mechanisms. In this study, we systematically investigated the reaction mechanisms governing conductive MOF formation and developed an environmentally benign, solvent-free, and cost-effective mechanochemical synthesis route. Conductive Co-, Ni-, and Zn-based MOFs were successfully synthesized using both manual grinding (mortar and pestle) and ball milling techniques within a remarkably short reaction time of 5 minutes. The resulting MOFs exhibited superior thermal stability and enhanced electrical conductivity compared to their solvothermally synthesized counterparts, underscoring the potential of mechanochemical synthesis as a sustainable and scalable strategy for fabricating conductive MOFs for advanced energy storage applications.

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Poster Presentation (P-17)

Metalloradical Catalysed Olefin Hydrogenation: A New Approach To Radical Hydrogenation

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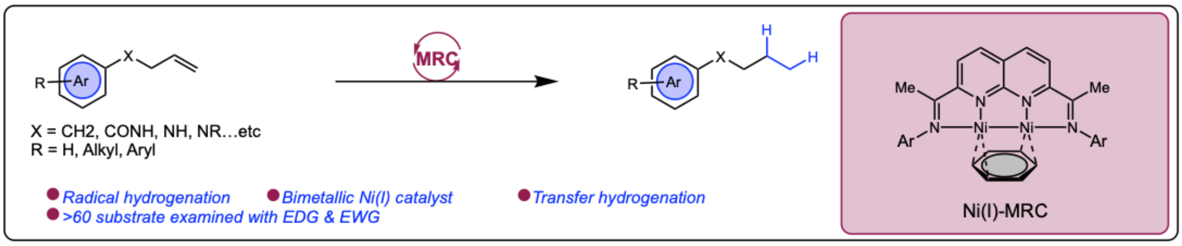
Abstract

Radical hydrogenation via Hydrogen Atom Transfer (HAT)/ Transfer Hydrogenation to alkenes is an increasingly important transformation for the formation of thermodynamically more stable alkane isomers. Current single-catalyst-based hydrogenation methods require a stoichiometric oxidant in addition to a hydride (H^-) source.[1] Hydrogenation based on radical, metal-catalysed hydrogen atom transfer (mHAT), *transfer hydrogenation* mechanisms offers an outstanding opportunity to overcome these difficulties, enabling the mild reduction of these challenging olefins with selectivity that is complementary to traditional hydrogenations with H_2.



X = CH2, CONH, NH, NR…etc
R = H, Alkyl, Aryl

- ● *Radical hydrogenation*
- ● *>60 substrate examined with EDG & EWG*
- ● *Bimetallic Ni(I) catalyst*
- ● *Transfer hydrogenation*

Scheme: Metalloradical(MRC) catalysed radical hydrogenation of olefines

Furthermore, it provides an opportunity for asymmetric induction through transfer hydrogenation using two different hydrogen sources.[2,3] Herein, we disclose the first report on metalloradical (MRC) catalysed radical hydrogenation of olefins using two distinct hydrogen sources ($NaBH_4$ & $Et_3N.3HF$). Control reaction confirms the generation of the H_2 molecule, which is further activated and subsequently donated to olefins via MRC-catalysed HAT. The bimetallic nature of MRC makes it even oxidant free. The mechanistic insights suggest the radical hydrogenation pathway. Together, this catalytic system allows us to hydrogenate different classes of molecules and introduces a new approach to radical hydrogenation.

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Poster Presentation (P-18)

Photoinduced Transitions in Transient Absorption Spectroscopy: Auger and Energy Transfer Dynamics in Mn-CsPbCl$_3$ Nanocrystals

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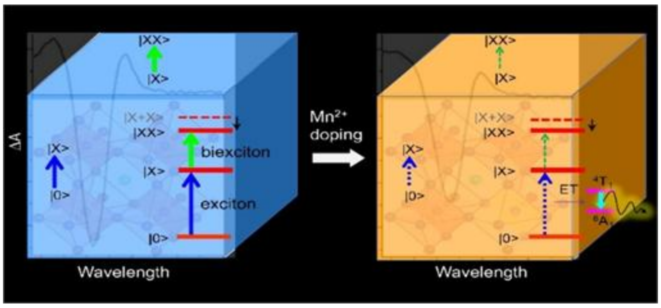
Abstract

We have reported photoinduced absorption features in Mn-doped CsPbCl$_3$ NCs using femtosecond transient absorption spectroscopy, focusing on both exciton bleaching and photoinduced absorption signals. We reveal that the photoinduced absorption features, often overlooked, originate from exciton-to-biexciton transitions and provide a more accurate measure of exciton-to-Mn energy transfer (ET) dynamics. Our analysis shows that ET time scales decrease with increasing Mn content, reaching ~112 ps for heavily doped samples, due to an efficient ET process. Additionally, biexciton Auger recombination and carrier trapping rates accelerate with Mn doping - a consequence of the increased ET phenomenon. These findings emphasise the importance of photoinduced absorption signals in transient absorption spectra for probing fundamental processes in doped perovskite NCs[1]. The developed model can be further extended to relevant sustainable systems, offering significant potential for advanced sustainable energy and optoelectronic applications.

Figure/Scheme:



Keywords: Mn-doping, CsPbCl$_3$ nanocrystals, exciton-biexciton, Auger recombination, transient absorption spectroscopy

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Poster Presentation (P-19)

Scalable Synthesis of N-Doped Carbon Catalysts for Acidic Oxygen Reduction Reaction

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Abstract

Biomass-derived carbon materials (BDCMs) are made from plant waste, such as: rice husks, coconut shells, corn cobs, sawdust, etc. Instead of relying on fossil fuels, we turn this waste into useful nitrogen-doped carbon catalysts, boasting a huge surface area brimming with pores. The structure helps boost the electrocatalysis in proton-exchange-membrane fuel cells (PEMFCs). The starting materials are renewable and often cheap or locally available, and both eco-friendly and cost-effective. BDCMs turn trash into high-performance, low-impact energy tech.[1] Here, we highlight tea waste as a low-cost precursor for nitrogen-doped porous carbon tailored for acidic oxygen reduction reaction (ORR), a key process in PEMFCs. Spent black tea leaves are carbonised and chemically/thermally activated to yield a micro/mesoporous framework, while intrinsic biomolecules act as *in situ* nitrogen sources. Structural analyses further confirm effective nitrogen incorporation and the formation of a well-developed porous nano architecture that facilitates mass transport. The resulting tea-waste-derived carbon exhibits strong ORR activity in acidic media, underscoring the potential of biomass waste valorisation to deliver high-performance, metal-free electrocatalysts, and advance efforts to develop sustainable energy-conversion technologies.[2]

Keywords: Tea waste, Waste to wealth, Solvent effect, Metal-free catalyst design, Oxygen reduction reaction, Nitrogen doping.

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Poster Presentation (P-20)

Synthesis of 1-Amino, 2-Acyl Cyclohexadiene via Metal Catalyst Free Csp^2-Csp^2(CO) Bond Formation

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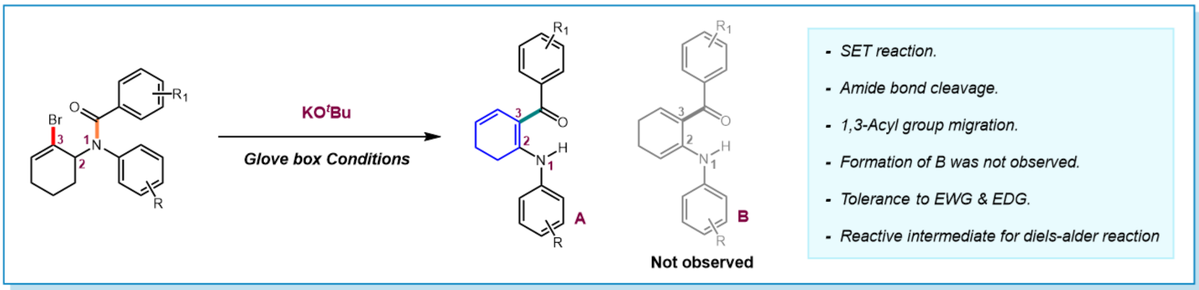
Abstract

Cyclohexadiene is an important core structure in numerous natural products, including alkaloids and terpenoids, and exhibits biological activities ranging from anti-bacterial to Anti-cancer.[1] Its derivatives also act as biosynthetic precursors for aromatic amino acids, vitamin K, and folate. Moreover, it serves as a highly reactive intermediate in the synthesis of analgesic drugs such as morphine and codeine,[2] as well as in the well-known Diels-Alder reaction. Herein, we report an efficient synthetic protocol to access a new class of cyclohexadienes from N-benzoyl bromo-alkene under transition-metal-free conditions. This strategy begins with the preparation of N-benzoyl bromoalkene from 1,2-dibromocyclohexene *via* C-N bond formation through nucleophilic substitution reaction.[3] Next, KO^{t}Bu mediated SET (Single Electron Transfer) promotes Intramolecular 1,3-acyl migration through amide bond cleavage, leading to Csp^2-Csp^2(CO) bond formation and selectively affords the 1-amino, 2-acyl, 1,3-cyclohexadiene product. The reaction shows broad tolerance towards both electron-withdrawing and electron-donating substituents. Our mechanistic studies confirmed the generation of a radical species via in-situ EPR (Electron Paramagnetic Resonance) study & radical trapping experiments, and controlled experiments highlighted the crucial role of the carbonyl group in driving the transformation.



- *SET reaction.*
- *Amide bond cleavage.*
- *1,3-Acyl group migration.*
- *Formation of B was not observed.*
- *Tolerance to EWG & EDG.*
- *Reactive intermediate for diels-alder reaction*

Figure: Synthesis of 1-amino, 2-acyl, 1,3-cyclohexadiene.

Keywords: Cyclohexadiene, Amide bond cleavage, Acyl migration, SET (Single Electron Transfer).

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Poster Presentation (P-21)

Understanding Gene Regulation by Virus-Encoded miRNA

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Abstract

The highly pathogenic avian Influenza type A, H5N1 virus produces microRNAs (miRNAs) that modulate host antiviral responses through gene silencing mechanism. The H5N1-derived miRNA, known as miR-HA-3p, specifically targets the host PCBP2 in the RIG-I/MAVS pathway, crucial for interferon production.[1] In this work, I examine the interaction of miR-HA-3p with the fragment of its host target PCBP2 using steady-state and single-molecule fluorescence techniques with the aim towards deciphering the molecular mechanism of the host gene regulation by the viral encoded miRNA.
First, we studied the salt (NaCl)-concentration dependent folding-unfolding of miR-HA-3p using Förster resonance energy transfer (FRET), which reports the distance dependent energy transfer from the 5'-donor fluorophore (FAM) to the 3' acceptor fluorophore (TAMRA). We observe that miR-HA-3p folds to a compact high-FRET structure with increasing salt concentration due to charge screening effect. Upon addition of unlabelled target PCBP2 mRNA to this FRET-pair labelled miR-HA-3p at physiological buffer conditions, we observe a significant decrease in FRET efficiency due to hybridization between miR-HA-3p and the target with a binding constant (K_d) of 6 nM. Similar measurements using fluorescence correlation spectroscopy (FCS) revealed an increase the diffusion time, with a $K_d \sim 5$ nM, confirming the transition from single-stranded miRNA to miRNA–mRNA duplex structures.[2] These studies provide a preliminary understanding of the folding-unfolding behaviour of miR-HA-3p and its affinity towards the target mRNA. Next, we plan to study the kinetic aspects of these folding/binding interactions using two-dimensional fluorescence lifetime correlation spectroscopy (2D FLCS) in cellular mimicking conditions to understand the gene silencing pathways using viral encoded miRNA.[3-4]

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Poster Presentation (P-22)

Electrochemical Synthesis of Graphene (Oxide) Colloids

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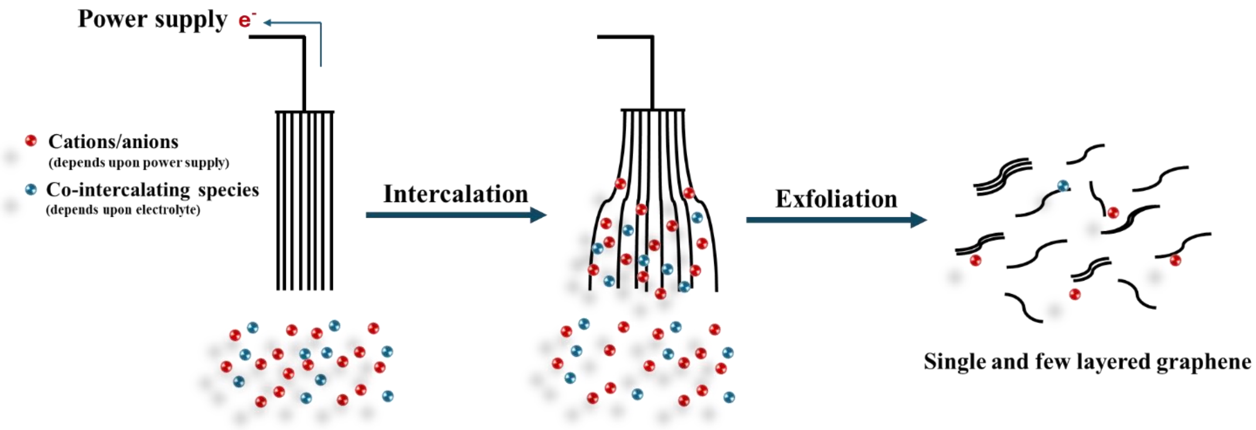
Abstract

To combat climate change by reducing CO_2 emissions in industrial processes pyrolysis of (bio)methane, a process that converts methane into turquoise hydrogen while capturing carbon as a solid by-product, is a promising approach.[1] These pyrolysis carbons may be a more sustainable alternative for mined graphite to produce graphene (oxide) materials for applications in energy storage and conversion, electronics, photonics, biomedical applications. Towards upcycling of pyrolysis carbons we first investigate electrochemical pathways with graphite flakes as a model system that are able to deconstruct carbon powders into graphene (oxide) colloids of tuneable size and composition.[2] A central focus of our approach is controlling exfoliation efficiency and tailoring the degree of oxidation and defect density within the graphene sheets by stepwise intercalation and exfoliation strategy. These factors strongly influence their functional properties such as electrical and thermal conductivity. Kinetic studies are being carried out in parallel to gain a mechanistic understanding of the exfoliation process through various electrochemical techniques, offering insights that can help extend this approach to a wide range of graphitic feedstocks. By leveraging advanced electrochemical techniques, this work seeks to enhance the economic and environmental sustainability of graphene production while promoting a circular economy. Ultimately, our research could lead to more accessible, eco-friendly graphene production methods, supporting both carbon management and energy conversion solutions for a greener, more sustainable future.

Scheme:



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Poster Presentation (P-23)

Engineering of Cathode and Electrolyte Additives Enables Highly Reversible Zn-ion Battery

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Abstract

Demand for high-efficiency energy storage and conversion devices is continuously increasing due to the ever-increasing human population and modernisation of society. Renewable energy technologies, such as fuel cells and batteries, have garnered significant attention for mitigating carbon emissions. Aqueous zinc-ion batteries are considered viable alternatives to lithium-ion batteries due to their built-in safety, adaptable structural options, and eco-friendly The primary categories of cathode materials found in zinc-ion batteries are manganese-based compounds, vanadium-based substances, Prussian blue analogues, organic compounds, transition metal sulfides and oxides, metal–organic frameworks (MOFs), covalent organic frameworks (COFs), and MXene-based layered materials. They encounter challenges related to zinc ion diffusion resistance and vanadium solubility. Transition metal sulfides and oxides also have high theoretical specific capacities, but their electrical conductivity and structural stability require improvement. The structures of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) can be designed to offer large specific surface areas; however, they suffer from low electrical conductivity and involve complicated synthesis methods. Enhancing the efficiency of zinc-organic batteries can be achieved by creating new organic molecules and polymer-based cathodes. Organic triazine-based framework shows commendable chemical stability and redox capability as a cathode material; however, they possess low electronic conductivity. To improve the conductivity, herein we proposed an in situ method of electronic conductive N-doped reduced graphene oxide(NrGO) to activate Poly (Imides-Triazine) based framework for a superior cathode material for a stable aqueous Zn-ion Battery. Another challenge in Zn-based batteries is the non-uniform deposition of Zn during plating, which results in dendrite growth. Due to the irreversible nature of the Zn anode, the lifetime of the battery is reduced. By engineering the electrolyte, the desolvation of Zn can be directed for the uniform deposition of Zn, and the local environment of the Zn anode can be modulated for the dendrite suppression. This approach enables the enhancement of zinc reversibility without compromising energy density or other additional processes. Herein, a dual electrolyte strategy has been employed by using two polar aprotic cosolvents, Dimethyl ethylene glycol dimethyl ether (DME) and Hexamethylphosphoramide (HMPA), in a 2M ZnSO4 electrolyte to regulate the solvation structure of Zn. Due to the presence of two cosolvents, the parasitic HER and Zn corrosion are suppressed. The abundant coordination sites of both electrolytes interact with the Zn ion, facilitating the reduction of the number of water molecules in the Zn solvation structure. The HMPA facilitated the deposition of zinc on the (002) plane, which has low surface energy and facilitates uniform growth. Simultaneously, DME will suppress the parasitic hydrogen evolution reaction (HER) to enhance the stability and reversibility of the Zn anode.

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Poster Presentation (P-24)

Efficient Access of 4(3H)-Quinazolinone via Carbon-Carbon Triple Bond Cleavage of Unactivated Alkyne

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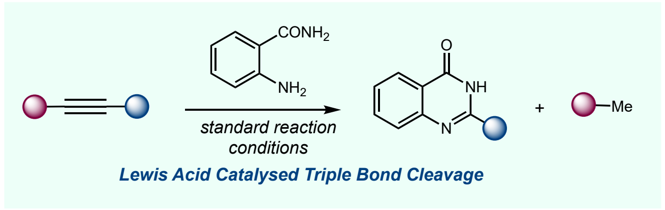
Abstract

A central goal of organic synthesis is the construction of complex, highly functionalized molecules from simple and readily available starting materials. While classical synthetic strategies have traditionally relied on functional-group interconversions and C–H bond functionalization of preassembled frameworks, an emerging and increasingly powerful paradigm is based on C–C bond cleavage, recombination, and strategic reorganisation. This approach enables fundamentally new disconnections and offers access to molecular architectures that are often difficult to achieve through conventional methodologies.[1] The challenge in C-C triple bond cleavage, recombination and transformation is limited due to the high bond dissociation energy (>200 kcal/mol).[2] Achieving this often requires **noble metal catalysts** and **stoichiometric non-renewable oxidants** to activate C≡C bonds, limiting it's applicability.[3]

On the basis of our continuous interest in the effective transformation of alkynes to afford easy access to 4(3H)-Quinazolinone and its derivates[4] which are found in more than 100 naturally occurring alkaloids.[5] Here, we report the Lewis acid-catalysed synthesis of 4(3H)-quinazolinone from phenyl acetylene and 2-aminobenzamides via carbon−carbon triple-bond cleavage using molecular oxygen (O_2) as the sole oxidant. This strategy enables the effective assembly of 4(3H)-Quinazolinone via C−N bond formation and aerobic C−C triple-bond cleavage. This method works well for both electron-deficient and electron-rich functional groups, and a total of 24 [4(3H)-Quinazolinone] compounds have been synthesised using it.



- *Efficient Cleavage of C-C Triple bond*
- *Efficient access of 5,6-membered heterocycles*
- *High functional group tolarence with yield up to > 78%*
- *Broad substrate scope (23 substrates)*
- *Under aerobic conditions*

Scheme: Lewis acid catalysed cleavage of C-C triple bonds.

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Poster Presentation (P-25)

Ni-Catalyzed New Method for One-Step Synthesis of 1,1-Aryl Ketone Cyclopropanes and 2,3-Dihydrofurans

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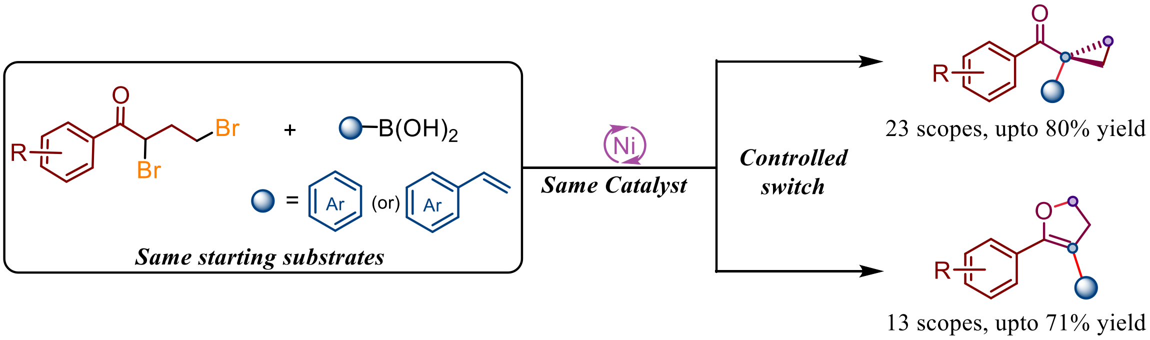
Abstract

In this article, we report a sustainable nickel-catalyzed platform for the selective synthesis of aryl-substituted cyclopropyl ketones and 4,5-substituted 2,3-dihydrofurans from simple precursors by precisely adjusting reaction conditions. This divergent methodology greatly broadens the synthetic toolbox for constructing structurally complex and highly functionalized frameworks sought after in drug discovery, agrochemicals, and advanced materials. Leveraging the environmental and economic benefits of earth-abundant nickel, this approach adheres to green chemistry principles, minimizes the use of precious metals, and is well-suited to large-scale manufacturing processes used in industry today. Systematic optimization reveals the factors that dictate product selectivity, enabling efficient access to diverse architectures from common starting materials with exceptional control and scalability. With operational simplicity, scalability, and sustainable alignment, this platform is attractive for academic and industrial applications, facilitating further innovative developments. Our findings lay the groundwork for expanding pharmaceutical and materials design via versatile, environmentally responsible rapid scaffold diversification. Full details, mechanistic insights, and applications will be presented at the conference.

Figure: One-pot Ni-catalyzed Suzuki cross-coupling and cyclization



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Poster Presentation (P-26)

Emissive Supramolecular Polymer from Diketopyrrolopyrrole Macrocycle

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Abstract

Supramolecular polymers have emerged as a versatile class of functional soft materials. Unlike conventional covalent polymers, they exhibit dynamic and adaptive behavior, enabling error correction, stimuli responsiveness, and hierarchical organization.[1] These unique features make supramolecular polymers promising candidates for applications in organic electronics, sensing, light-harvesting, photocatalysis, and biomimetic materials. Despite remarkable progress, precise control over the self-assembly of supramolecular polymers remains challenging due to inherent pathway complexity arising from multiple competing aggregation routes and shallow energy landscapes.[2] Even small variations in molecular structure or external conditions can lead to kinetically trapped states or uncontrolled polymer growth. Addressing this pathway complexity is therefore crucial for achieving predictable structures and functions. In this context, living supramolecular polymerization (LSP) has emerged as an advanced strategy to regulate supramolecular growth with high precision.[3] By suppressing spontaneous nucleation and enabling seeded growth, LSP allows controlled length, dispersity, and morphology. In this direction, emissive supramolecular polymers derived from π-conjugated chromophores are of particular interest because of their potential applications in imaging and optoelectronic devices. However, many such polymers are non-emissive despite the emissive nature of their monomers, owing to aggregation-induced fluorescence quenching. In contrast, *J*-aggregated supramolecular polymers exhibit bright emission, making them especially attractive for photonic applications, including artificial light-harvesting systems. Here, we will present a diketopyrrolopyrrole-based macrocycle that displays pathway complexity and undergoes living supramolecular polymerization via a J-aggregation, which results in bright red emission, highlighting the potential of this system for optoelectronic and imaging applications.[4]

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Poster Presentation (P-27)

Heavy-Atom-Modulated Pentacyclic Pyryliums: Tunable Platforms for Bioimaging and Diagnostics

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Abstract

Pentacyclic pyrylium fluorophores offer rigid scaffolds with tunable electronics for bioimaging applications, inspired by successful heteroatom engineering in rhodamine dyes that revolutionized optical properties and biological utility. Pentacyclic pyrylium fluorophores offer rigid scaffolds with tunable electronics for bioimaging applications, inspired by successful heteroatom engineering in rhodamine dyes that revolutionised optical properties and biological utility. Here we report, for the first time- heteroatom (O, NMe, NH, S, Se) incorporation into the pentacyclic pyrylium core, enabling predictable emission tunability from blue-shifted visible emissions to pronounce near-infrared bathochromic shifts (>100 nm) via precise electronic structure and band-gap modulation. Here we report, for the first time- heteroatom (O, NMe, NH, S, Se) incorporation into the pentacyclic pyrylium core, enabling predictable emission tunability from blue-shifted visible emissions to be pronounced near-infrared bathochromic shifts (>100 nm) via precise electronic structure and band-gap modulation. Heavier chalcogens (S, Se) enhance intersystem crossing through the heavy-atom effect, boosting reactive oxygen species generation, while optimizing lipophilicity, charge distribution, biocompatibility, cellular uptake, and organelle-specific localization. Density functional theory calculations confirm heteroatom-driven orbital hybridization and charge redistribution as the origin of this versatility. These platforms exhibit superior photostability, brightness, and performance in live-cell imaging, establishing heavy-atom-modulated pentacyclic pyryliums as powerful tools for fluorescence sensing, bioimaging, and advanced diagnostics.

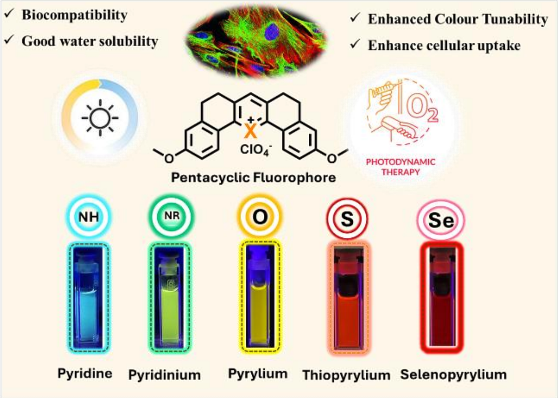

Figure: Heteroatom engineering-driven modulation of pentacyclic pyrylium fluorophores for theranostic applications.

Figure: Heteroatom engineering-driven modulation of pentacyclic pyrylium fluorophores for theranostic applications.

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Poster Presentation (P-28)

Understanding the biophysical properties of microRNA-21 (miR-21) at the single-molecule level

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Abstract

MicroRNAs (miRNAs) are small, non-coding RNA molecules that regulate gene expression post-transcriptionally by binding to complementary messenger RNAs (mRNAs), leading to their degradation or translational repression. They play essential roles in cellular homeostasis, influencing processes such as cell growth, differentiation, and apoptosis. Dysregulation of miRNAs can lead to pathological conditions, including cancer, where impaired apoptotic regulation enables uncontrolled cell proliferation.[1] Among various miRNAs, microRNA-21 (miR-21) is one of the most studied oncogenic miRNAs, consistently overexpressed in cancers like breast, liver, and colorectal. miR-21 promotes cancer by suppressing tumour-suppressor genes such as PTEN, FOXO1, BTG2, etc.[2] While previous research has focused on identifying these targets and correlating miR-21 levels with cancer progression, the biophysical properties of miR-21 in varying physicochemical conditions and its interaction with these targets remain poorly understood.

In this work, we study the folding-unfolding properties of a Förster Resonance Energy Transfer (FRET) pair labelled miR-21 and its interaction with three unlabelled mRNA targets, PTEN, FOXO1, BTG2, with steady-state fluorescence spectroscopy and fluorescence correlation spectroscopy (FCS). NaCl-concentration dependent folding-unfolding studies on miR-21 at different pH (6.0, 7.4 and 8.5) show that miR-21 adopts a compact high FRET structure at high salt concentrations and lower pH, due to charge screening effect by NaCl and charge neutralization on RNA, respectively. The binding studies with the three targets at pH7.4 reveal that miR-21 transitions from a fast diffusing, compact high-FRET conformation to a relatively slow diffusing, low-FRET open conformation in the miRNA-target mRNA complex however with different binding affinities. The differences in the binding affinities are attributable to the strengths of the miRNA-target mRNA base-pair interactions. These findings are a step towards understanding the dynamic structural diversity of miR-21 and its role in regulating apoptosis and cancer progression through the interaction with different targets.

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Poster Presentation (P-29)

Metal- and base-free spirocyclization of alkylidene oxindoles via mechanochemically generated nitrile imines as 1,3-dipoles

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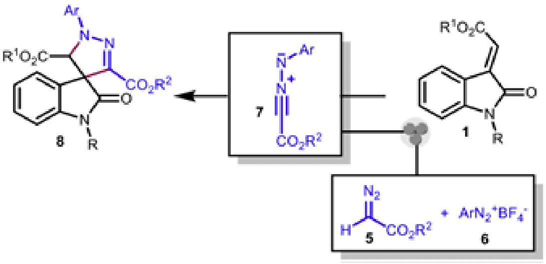
Abstract

Spirocyclic oxindole scaffolds are privileged structures in medicinal chemistry, yet their synthesis often requires hazardous solvents or metal catalysts [1]. We report an efficient, solvent-free mechanochemical protocol for the synthesis of functionalized 2'-aryl-2',4'-dihydrospiro[indoline-3,3'-pyrazol]-2-ones [2]. Utilizing high-frequency ball milling, we successfully facilitated the [3+2] cycloaddition of alkylidene oxindoles with nitrile imines, generated *in situ* from ethyl diazoacetate and aryl diazonium tetrafluoroborates without pre-functionalization [3]. Optimized conditions using a stainless steel jar assembly at 70 Hz afforded the desired spirocyclic scaffolds in excellent yields (up to 87%) within just 30 minutes. This metal- and base-free strategy demonstrates broad substrate scope and was successfully scaled up using a DYNO®-MILL bead mill, offering a greener alternative to traditional solvothermal methods [4].



Scheme: Summary of our work.

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Poster Presentation (P-30)

Z-Selective Synthesis of β-Fluoro Michael Acceptors via Ring Opening of 5-Membered Cyclic Molecules

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Abstract

Life on Earth produces fluorinated carbon compounds far less frequently than other halocarbons, which are more common in various natural processes. Nonetheless, the distinct properties of the fluorine atom make it a crucial component across multiple fields, including medicinal chemistry, agrochemical development, and materials science. Specially introduction of fluorine into organic molecules can significantly modify their physicochemical properties, enhancing their effectiveness and functionality.[1] Despite progress in the field, incorporating fluorine into compounds remains challenging due to the complexity of its chemistry and the need for precise conditions. In this study, we present a silver-mediated approach for the selective fluorination of a puckered bicyclic heteroatom-containing compound.[2] This method yields highly selective β-fluorinated substituted unsaturated ketones, achieved through a process known as deoxydesulfuration. To understand the reaction mechanism in detail, both experimental and theoretical tools have been utilised.[3]

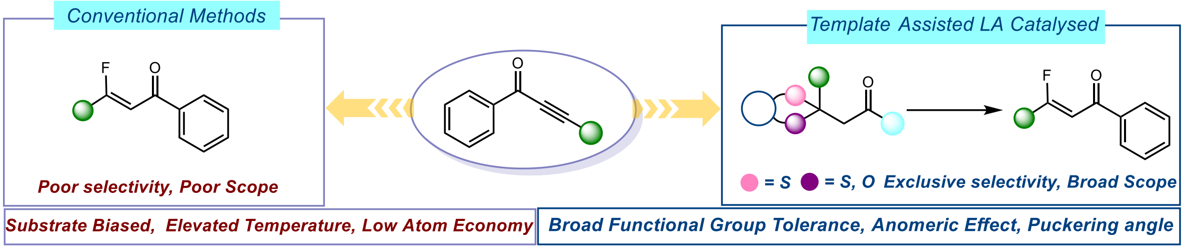

Figure: Lewis Acid Catalysed Fluorination of 5-Membered Cyclic Molecules

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Poster Presentation (P-31)

Understanding dissolution mechanism of oxide perovskites and activity tuning for O_2 evolution by surface doping

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Abstract

Oxygen evolution reaction represents the major bottleneck in electrochemical water splitting. Development of efficient electrocatalysts from earth-abundant materials is essential.[1,2] This study reports a design principle for tuning the catalytic efficiency and stability of perovskite oxides, focusing on $SrMnO_3$, $SrFeO_3$, $SrCoO_3$, and $SrNiO_3$ through B-site surface doping with Mn, Fe, Co, and Ni metal ions. Owing to multiple active sites and tunable oxidation states, these oxide surfaces exhibit a considerable reduction in thermodynamic overpotential (η_{TD})[3,4] upon doping. Such trends are consistent with recent advances in thermodynamic and kinetic modeling of electrocatalytic reactions using first-principles approaches.[4] The dissolution free energy calculations are performed across a wide pH window (acidic to alkaline) and oxidative potentials to determine the Pourbaix stability and surface dissolution pathways. We find that $SrCoO_3$ and $SrNiO_3$ show the highest stability on doping with different transition metal atoms.

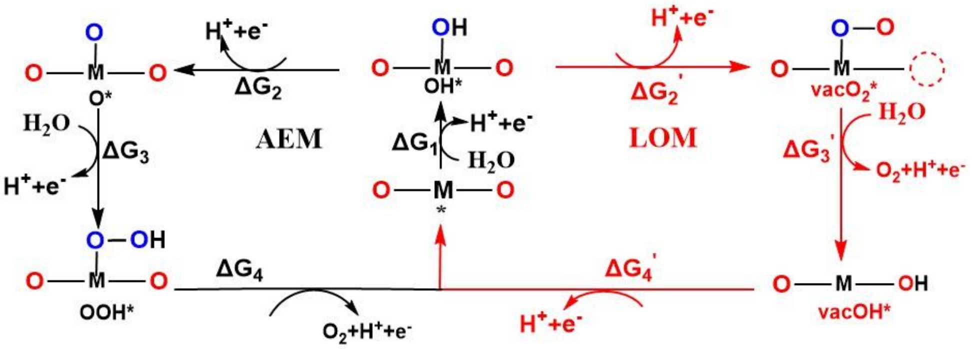

Figure 1. The adsorbate evolution mechanism (AEM) and the lattice oxygen mechanism (LOM) are illustrated: black for AEM and red for LOM. Each step follows proton-coupled electron transfer, with free-energy changes (ΔG_i) indicated.

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Poster Presentation (P-32)

Revisiting the Role of Solvent-induced MOF Size Variation and Single-atom Catalysts Development for Oxygen Electrocatalysis

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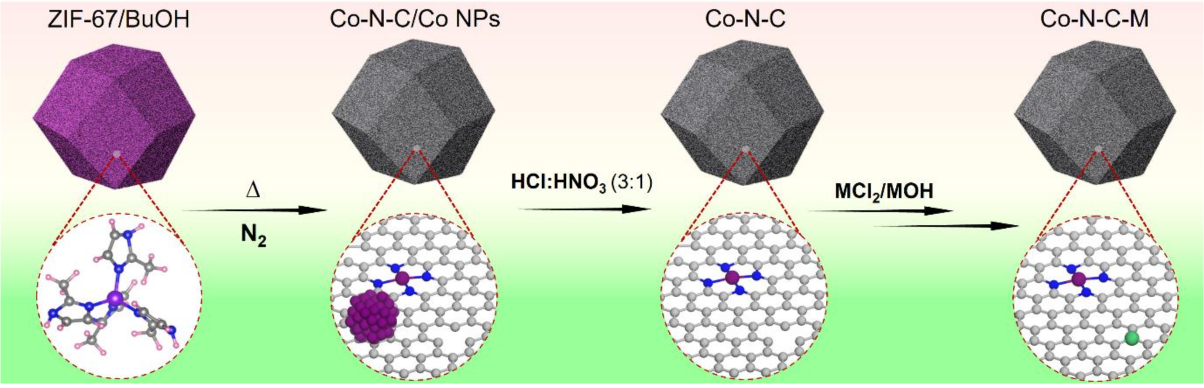
Abstract

Enhancing the kinetics and selectivity of the oxygen reduction reaction (ORR) and the oxygen evolution reaction (OER) is crucial for advancing energy devices, such as fuel cells and PEM water electrolyzers.[1] Single-atom catalysts (SACs) featuring M–N_4/C structures have shown exceptional ORR/OER performance.[1,2] Here, we present a high-efficiency atomic cobalt (Co) catalyst derived from zeolitic imidazolate frameworks (ZIF-67) without incorporating zinc (Zn) as a co-dopant. In addition, the impact of the solvent dielectric constant has been demonstrated to control the tunable catalyst particle sizes ranging from 400 to 1200 nm. This method enables size tuning without altering chemical composition, thereby increasing the density of PGM-free active sites, similar to the effect seen in Pt nanoparticles. Using atomically dispersed Co catalysts, we tracked the formation of active sites by linking ORR performance to chemical transformations during pyrolysis up to 1000 °C. Despite this progress, differences in ORR performance persist under acidic versus alkaline conditions. Furthermore, the electronic modification is made between the first and second coordination spheres to modulate the deactivation steps. The enhanced ORR activity of atomic Co catalyst design offers tunable structure, improved diffusion, and defined active sites, positioning it as a strong platinum-group-metal-free candidate for future proton exchange membrane fuel cells (PEMFCs).



Scheme: Step-wise synthesis route for M–N_4-M/C catalyst development.

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Poster Presentation (P-33)

Catalyst-Free Electro-Photochemical Hydroalkylation Of N-Aryl Maleimides *via* Alternate Electrode Electrolysis: A Sustainable Route To N-Aryl Succinimides with Quaternary Center

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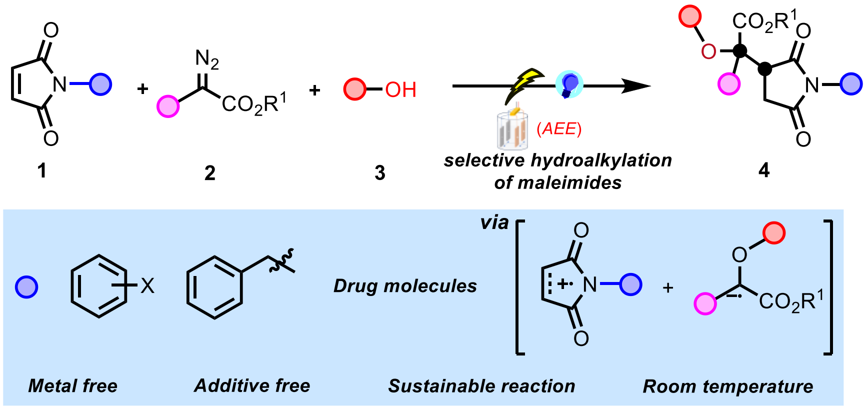
Abstract

In this article, we have reported a dual electrochemical-photochemical platform that enables selective hydroalkylation of N-aryl maleimides for the construction of C4 functionalized N-aryl succinimides in the presence of alcohol (as a solvent) and aryl diazo esters. Succinimides are valuable five-membered nitrogen-containing heterocycles widely recognized for their presence in pharmaceuticals, agrochemicals, and natural products.[1] We have developed Alternate electrode Electrolysis (AEE) technique which selectively promotes electrochemical reduction of *N*-aryl maleimides which undergoes cyclopropanation with a blue light generated carbene, subsequent ketyl radical mediated ring opening and electro-oxidative nucleophilic attack by alcohol afford the densely substituted hydroalkylated succinimide derivative. The protocol showcases high functional group tolerance, affording over 26 structurally diverse N-aryl succinimide derivatives, including the late-stage functionalization of aromatic amine-containing pharmaceutical scaffolds. A gram-scale synthesis underscores the scalability and operational simplicity of the process. Control experiments highlight the orthogonal yet complimentary nature of the activation modes and provide mechanistic evidence supporting a stepwise paired electrolysis process aided with photochemical carbene generation pathway.



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Poster Presentation (P-34)

Design of Amino-Functionalized Metal-Frameworks for Efficient Iodine Capture towards Nuclear Waste Remediation

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Abstract

In this article, we have reported that the management of radioactive nuclear waste is of great importance due to its long-term hazardous environmental health effects, where radioactive iodine is one of the most prominent in this category, holding a significant share amongst the radioactive contaminants. In this work, we report the green synthesis of a new, zirconium-based, mixed linker metal-organic framework for the adsorption and removal of radioactive iodine from nuclear waste. A one-pot solvothermal synthesis method was employed using two bio-derived acidic amino acids as linkers in varying ratio (10:90 to 90:10), harnessing the properties of both the linkers by the mixed-linker effect compared to the single-linker MOFs. Structure characteristics were evaluated using XRD, IR, TGA and BET which confirmed the successful formation of crystalline, thermally stable and porous frameworks. Among the series the MOF synthesized with a 60:40 linker ratio exhibited significantly enhanced surface properties and demonstrated the highest iodine adsorption efficiency, outperforming both pure single-linker MOFs. The superior performance can be attributed to the synergistic effect of dual linkers, which optimized pore diameter and adsorption sites. This study highlights an environmentally friendly approach to design functional MOFs and establishes a promising platform to overcome nuclear waste challenges.

Keywords: Metal-Organic Framework, Green synthesis, Radioactive waste management.

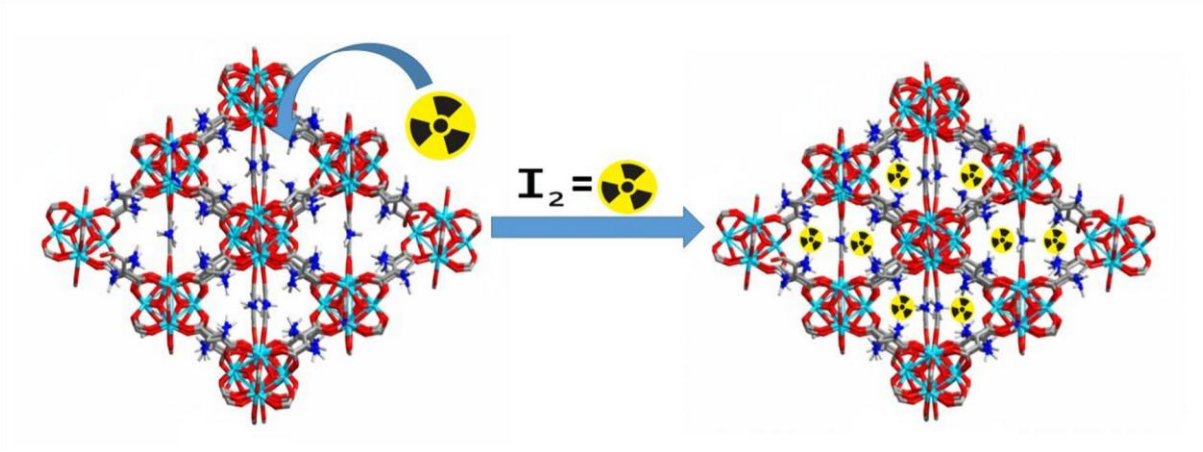

Figure: Schematic representation of I2 removal via synthesized MOF.

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Poster Presentation (P-35)

Unveiling Alternate Electrodes Electrolysis in Electro-Photochemical and Electro-Organic Synthesis

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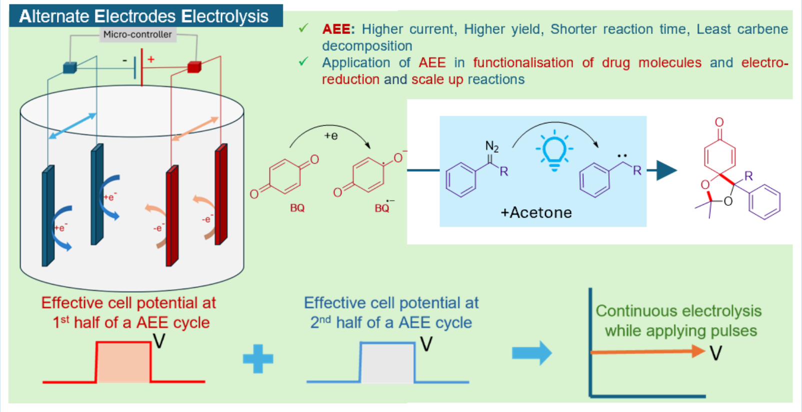
Abstract

Electro-photochemical organic synthesis is a rapidly growing field. Recently, technological advancement has contributed significantly to improve electro- and photolytic organic transformations in terms of energy efficiency and productivity. Herein we have introduced a new technique, called alternating electrodes electrolysis (AEE) in electrosynthesis which in combination with blue LED demonstrated an interesting three-component reaction with aryl diazoesters, 1, 4- quinones and acetone to synthesize ketal-functionalized 1,4-quinones. The setup of AEE consists of two pairs of cathode-anode compared to the conventional set up of one pair. Each pair would be in polarized or in a resting stage with preset interval of choice. This would maintain an overall continuous potential resulting in maximum current and facilitate the mass transport, thus increasing overall efficiency of the reaction. AEE offers efficient utilization of photochemically generated transient carbenes. We extended AEE application in paired photo-electrolysis reactions for the late-stage functionalization of bioactive molecules and pharmaceutical agents. As an application of AEE in electrosynthesis (without light) we demonstrated efficient hydroxylation of fluorinated benzene and reduction of benzonitrile to benzyl amine. The amalgamation of AEE with blue LED contributes to sustainability and we believe it holds great promise in the field of electro-photochemical organic synthesis.



Alternate Electrodes Electrolysis

- ✓ **AEE:** Higher current, Higher yield, Shorter reaction time, Least carbene decomposition
- ✓ Application of AEE in functionalisation of drug molecules and electro-reduction and scale up reactions

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Poster Presentation (P-36)

ELECTRO-PHOTOCHEMICAL C3-FUNCTIONALIZATION OF NH-INDOLES

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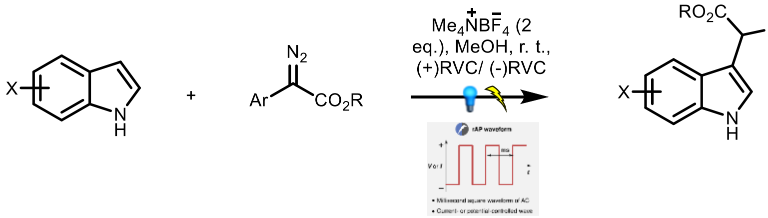
Abstract

Electrochemical synthesis offers a sustainable strategy for generating reactive intermediates under mild conditions. This ongoing study investigates rapid alternating polarity (rAP) electrolysis in methanol, a polar protic solvent, with emphasis on mechanistic control and synthetic potential. The rAP technique employs millisecond-scale alternating waveforms that suppress the accumulation of long-lived radical ions, leading to improved reaction selectivity [1].

Under rAP electrolysis conditions, transient indole radical cations are formed and stabilized through hydrogen-bonding interactions between methanol and the N–H group [2]. Simultaneously, the acceptor-derived electrophile (ADE) undergoes photoactivation or partial electrochemical reduction to generate a neutral or weakly radicalized carbene-like species. The rapid polarity switching enables controlled radical generation and promotes open-shell radical–radical coupling pathways.

Preliminary results suggest that rAP electrolysis provides superior control over reactive intermediates compared to conventional direct current methods. This work highlights the potential of rAP electrochemical strategies for efficient and selective radical-mediated organic synthesis [1,3].



Scheme 1: Our method, and literature precedents for preparing C3-arylated indoles.

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Poster Presentation (P-37)

Tuning Single-Atom Catalysts for Carbon Dioxide Reduction Reaction

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Abstract

Over the past few years, the electrochemical CO_2 reduction has been an emerging and promising solution to maintain the global carbon balance. The noble metal surfaces, such as Au, Ag, have been found to show superior activity for CO_2 to CO product. Cu is a unique metal that shows activity for reduction products beyond the two-step CO formation (Both C_1 and C_2 products). However, the Cu surface shows low product selectivity. These catalysts would be formidable for industrial-scale utilizations due to their expensive nature and less product selectivity. Therefore, stable electro- catalysts with high activity and selectivity are urgently needed. Here, we show an efficient strategy to enhance the activity of single-atom catalysts (SACs) for post-CO products (Methanol and Methane). To probe the local chemical bonding and structural properties of SACs, we considered 3d transition metals (Group VIII & IX) with porphyrin ligand frameworks. Using the density functional theory calculations and grand canonical potential simulations, we formulate an activity volcano for possible reduction products with the help of thermodynamic and kinetic analysis. We will propose a catalytic design principle by understanding chemical bonding nature, orbital interactions, and their electronic properties.

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Poster Presentation (P-38)

Deep Eutectic Solvent Mediated Ionic Cascades: Direct Access to Azaindazoles and Related Fused Heterocycles from Diverse N-Arenes

Yashika Tyagi,[1] Subhankar Bera,[1] Soumil Sen,[2] Renu Bhati,[1] Biswajit Guchait,[1] Sriram Dharmarajan,[2] Tanmay Chatterjee,[2] Ludovic Gremaud*,[3] and Subhabrata Sen*,[1]

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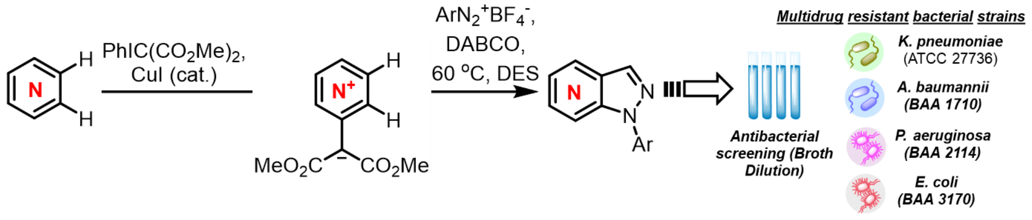
Abstract

In this article, we have reported a sustainable strategy for the direct C–H functionalization of pyridines, quinolines, isoquinolines, quinoxalines, pyrimidine and pyrazine to access N-aryl-7-azaindazoles and related fused azaheterocycles. Heteroarene ylides, generated from readily available precursors, react with aryl diazonium tetrafluoroborates in presence of DABCO through an ionic cascade of nucleophilic substitution, intramolecular SNAr, electrocyclization, and rearomatization. Deep eutectic solvents (DES) serve as efficient and green media, stabilizing diazonium salts, mitigating safety concerns, and enabling these transformations under mild conditions at 60 °C with broad substrate scope. This protocol establishes DES as a safe, scalable, and environmentally benign platform for heteroarene editing and late-stage diversification of drug-like molecules.[1-3] Some of the final compounds demonstrated moderate antibacterial activity against antibiotic resistant gram-ve bacteria.



Scheme: Summary of our work

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Poster Presentation (P-39)

Enantioselective C(sp^3)-H Chlorination by Ni(II)-CTAmide complex

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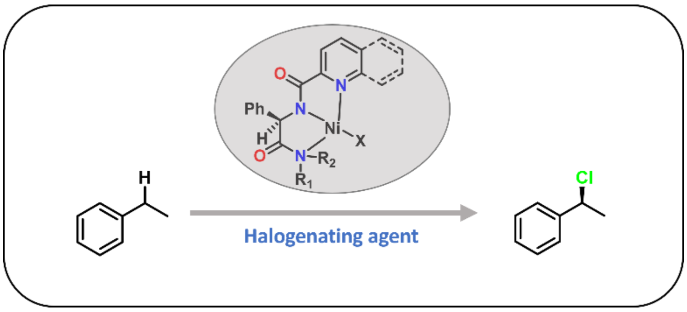
Abstract

Chiral chlorinated organic molecules serve as indispensable intermediates in pharmaceuticals, agrochemicals, flavors, and fragrances,[1] where the stereochemistry critically governs biological activity.[2] In this work, we describe the design of a novel tridentate asymmetric ligand incorporating two carboxamide nitrogen donors and an additional coordinating site. The carboxamide nitrogens provide both σ- and π-donation, stabilizing higher oxidation states of the coordinated metal. Nickel was chosen as the catalytic center owing to its low toxicity, earth abundance, and versatility in asymmetric catalysis.[3] The resulting ligand–Ni complex enabled the development of an efficient protocol for asymmetric chlorination, with ethylbenzene employed as the model substrate. The reaction afforded (R)- and (S)-(1-chloroethyl)benzene with 92% enantiomeric excess (ee), favoring the R-enantiomer. Ethylbenzene bearing electron-donating substituents afforded high enantioselectivities (85–95% ee), whereas electron-withdrawing substituents predominantly yielded racemic mixtures.



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Poster Presentation (P-40)

Multiscale Computational and Experimental Insights into Mutation-Induced Structural Instability and Cofactor Binding Perturbations in Valosin-Containing Protein

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Abstract

Valosin-containing protein (VCP) is a multifunctional AAA+ ATPase that plays a central role in cellular proteostasis, including ER-associated degradation (ERAD), ubiquitin-dependent protein turnover, and organelle quality control [1]. Disease-associated mutations within its N-terminal domain, notably the Arg95Gly (R95G) substitution, have been linked to multisystem proteinopathies such as inclusion body myopathy with Paget's disease and frontotemporal dementia (IBMPFD) and amyotrophic lateral sclerosis (ALS). However, the structural & molecular basis by which these mutations impair VCP function remains unexplored [2]. Here, we utilized an integrated computational and experimental approach to delineate the structural and dynamic effects of the R95G mutation on the VCP N-domain and its interaction with the gp78 cofactor peptide. Our workflow combined AlphaFold3-based structural modeling, protein-peptide docking, and multiscale molecular dynamics simulations employing both all-atom and coarse-grained MD simulations. Detailed analyses of physicochemical properties, intermolecular contacts, and free-energy landscapes revealed that the mutant VCP-N-gp78 complex exhibits reduced structural stability, decreased compactness, and weakened intermolecular interactions compared to the wild-type complex. Consistently, MM/PBSA-based binding free energy analyses indicated a substantial loss in binding free energy and altered residue-specific energetic contributions upon mutation. These computational findings were further experimentally validated through recombinant expression and purification of the VCP N-domain, followed by biophysical characterization and isothermal titration calorimetry, which confirmed diminished binding affinity and reduced stability of the mutant complex. Collectively, this study provides mechanistic insight into mutation-driven VCP dysfunction and establishes a robust framework for exploring therapeutic interventions in VCP-associated proteinopathies.

Keywords: Valosin-containing protein, AlphaFold3, protein-peptide docking, molecular dynamics simulations, therapeutic interventions

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