



International Conference on
**Progress and Challenges in
Modern Day Science
(PCMDS-2021)**



17 & 18 June, 2021

Book of Abstracts



Organized by

Department of Chemistry

B. Borooh College

In Association with

Assam Science Society

International Conference on
Progress and Challenges in Modern Day Science
(PCMDS-2021)

Date: 17 & 18 June, 2021
Website: www.seminarchembbc.com

Abstract Book



Organized by
Department of Chemistry, B. Borooah College,
Assam, India



In Association with
Assam Science Society
Assam, India

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ড° হিমন্ত বিশ্ব শর্মা
Dr. Himanta Biswa Sarma



মুখ্যমন্ত্রী, অসম
Chief Minister, Assam



Dated Dispur, the 14th June, 2021

MESSAGE

I am glad to know that the Department of Chemistry, B. Borooah College, Guwahati in association with Assam Science Society is organising an International Conference on **Progress and Challenges in Modern Day Science** on virtual mode on 17 and 18 June, 2021. An Abstract Book is being published to mark the event.

Science is the pillar of development in the modern-day society. Elevating the knowledge and skills of our younger generation on science, holds the key of our development. I hope the international conference being organised on the theme is of paramount importance in transforming our scientific knowledge to propel growth and development. I moreover, hope that the deliberations in the conference will be able to chart out an agenda to negotiate with the challenges of the modern-day science.

I convey my best wishes to the organizer and the editorial team of the Abstract Book resounding success in their endeavour.


(Dr. Himanta Biswa Sarma) 14/6



GAUHATI UNIVERSITY
GOPINATH BARDOLOI NAGAR:: ASSAM:: INDIA

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Prof. (Dr.) Pratap Jyoti Handique

Vice Chancellor
Gauhati University



Message

It is my pleasure to know that an International Conference titled “Progress and Challenges in Modern Day Science [PCMDS-21]” is being organised by Department of Chemistry, B Borooah College on 17th and 18th June 2021 in virtual mode. An Abstract Book will be published incorporating the abstract of papers presented in the e-conference. I appreciate the B. Borooah College fraternity and particularly the Department of Chemistry for organizing this e-conference on a broad subject of importance amidst Covid-19 emergency.

It is a well-known perception that modern science is a process of understanding the natural and physical world, based on recognizable evidence or proof, interpretation, and repeated testing. Various schools of thought opined that the process in the scientific method involves making hypotheses, deriving prediction or calculation from them as logical consequences, and then carrying out experiments or empirical observations based on those predictions. These hypotheses are then tested by scientists conducting experiments or other form of studies. The modern science has been growing and progressing for last about 500 years since the days of Galileo within these basic philosophical framework and practices. It is worth mentioning that Albert Einstein called Galileo the “father of modern science.” Until the time of Galileo Galilei, the Earth was thought to be the center of the universe. Galileo's mathematics based objective observations ignited one of the foundations of modern science. However, according to several historical notes the earliest dates for the birth of modern science range from the High Middle Ages in 1277 through the 17th century. Some historians cite a second scientific revolution to have occurred in the early 20th century with the advent of quantum physics.

Progress in science has also been defined in various ways by the scientists and institutions. According to a recent definition - “science makes progress when it develops concepts, typologies, frameworks of understanding, methods, techniques, or data that make it possible to uncover phenomena or test explanations of them”. Thus, knowing where and how to look for discoveries and explanations is an important type of scientific progress. We have witnessed incredible progress in science particularly during the 19th and 20th centuries. Besides producing in-depth knowledge and developing techniques on characterization, processing, modification, reconstruction and transformation of the total physical world, science has also made meticulous progress on almost all aspects of biological world. However, the increasing scientific work has caused diverse impact on the physical, biological and human's social environment of the globe. Science is facing challenges from various angles of its progress and as well as applications.

I do hope this International e-conference will make out significant objectives and work-plan to identify the progress and challenges of science in recent days. I wish the conference a success and expect that the Abstract Book will include good amount of significant research outcome.

Prof. (Dr.) Pratap Jyoti Handique
Vice Chancellor
Gauhati University

Date: 14-06-2021



COTTON UNIVERSITY

Panbazar, Guwahati-781001, Assam, India

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Date: 14th June, 2021



Message from Vice-Chancellor, Cotton University

I am happy to learn that **B Borooh College** in association with **Assam Science Society** is organizing an International Conference on **'Progress and Challenges of Modern-Day Science'** on June 17 and 18, 2021 in virtual mode.

Every educational institution has a responsibility to produce human resources to meet society's future needs. More importantly, the college also has a responsibility to prepare each individual student for the challenges they will face in their personal and professional lives. In fact, the New Education policy, 2020 of UGC lays particular emphasis on the development of the creative potential of each individual student. In the research space, this is becoming more and more challenging due to the increasingly interdisciplinary nature of science today. To become a research scientist a young researcher in Chemistry must also know a lot about Biology, Mathematics, Medicine, etc., in addition to his/her expertise in their primary subject.

Fortunately, the world is now very small as a result of fast communication systems, which opens the door to a vast amount of knowledge via online courses. It will be the responsibility of each teacher to be a guide by encouraging the students to enroll in Massive Open Online Courses (MOOC) so that they will be exposed to ideas beyond their main area of interest. The synthesis of learnings from a zone of inter-related subjects will form the bedrock upon which the careers of the next generation of students will be built.

I hope this conference and other similar workshops/online courses will expose our students to the modern world of science and will help humankind in solving the unsolved mysteries of the living world in a scientific way.

With best wishes

Prof B C Goswami

Vice Chancellor, Cotton University

MADHABDEV UNIVERSITY

(A State University established under the Assam Act No. XXXV of 2017)
Narayanpur, P.O. Dikrong-784164, Dist. Lakhimpur, Assam

Prof. (Dr.) Dibakar Chandra Deka M.Sc., M.Tech., Ph.D., DTIT, D.Sc., FRSC
Vice-Chancellor



Message

I am glad to know that the Department of Chemistry, B. Borooah College, Guwahati is planning to organize an international conference on ‘*Progress and Challenges in Modern Day Science*’. As informed the conference would be held on virtual mode necessitating no physical presence. Online conferences are as good as conventional ones as far scientific discussions and knowledge sharing are concerned. Through such conferences we can save a lot of valuable time, also such meetings involve less monetary cost. I convey my best wishes for the grand success of the two-day event on 17 and 18 June 2021. It is pleasing for me that BB College in general, and the Department of Chemistry in particular, are active as usual even in these days of lock down due to COVID-19 pandemic. I, not only wish them grand success but also congratulate all the faculty members and the staff for the endeavor. Less than a year ago the Department of Chemistry organized another national seminar in 2020. I wish the department would continue to play the role model for others.



(D. C. Deka)

Prof. B. K. Das M.Sc. (GU), Ph.D. (IISc)

Vice-Chancellor



MESSAGE

I am indeed very happy to learn that the *International Conference on Progress and Challenges in Modern Day Science* is being organized in the virtual mode by the Department of Chemistry, B. Borooah College, Guwahati on the 17th and 18th of June, 2021. It is heartening to note that the conference is being held amidst the challenging times that we all are currently passing through. A tiny microorganism has shaken the spacefaring humanity to the core so much so that not even scientists are sure about the extent of protection to be accrued from the vaccines meant to prevent attacks by the novel coronavirus. This underlines the importance of remaining steadfast in our engagement with research and other academic activities so that we are able to prepare ourselves for facing this as well as other calamities such as cyclones and floods that are tormenting us at an alarming frequency.

With the participation of eminent scientists from India and abroad who will present their research in the conference, I am sure the participating teachers as well as students of the region will get a great opportunity to enrich themselves with knowledge regarding developments in various frontiers in the sciences. I wish the organizers a grand success in their endeavour.

With best wishes,

Birinchi K. Das

14-06-2021

(BIRINCHI KUMAR DAS)

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বি. বৰুৱা কলেজ অধ্যক্ষৰ কাৰ্যালয় : গুৱাহাটী-৭, অসম

স্থাপিত : ১৯৪৩ চন

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Message

It gives me immense pleasure to welcome all the esteemed speakers and participants to the virtual **International Conference on Progress and Challenges in Modern Day Science (PCMDS-2021)** being organised on 17-18 June 2021 by the Department of Chemistry, B Borooah College in association with Assam Science Society.

This conference aims to bring scientists from different parts of the globe to a common platform where they can share and exchange ideas. The conference aims to celebrate the progress and dwell on the challenges of science. The virtual mode, a sign of technological progress, has been a boon in the times that we are living at present. The conference has been possible because of it. The response of the participants has been overwhelming.

The world is facing difficult times. Many have lost their near and dear ones because of the havoc of Covid-19. But as they say the show must go on. It is the human spirit that keeps us all going against all odds. To organise a conference at times of lockdown and curfew is a herculean task and I take this opportunity to appreciate the efforts of the Department of Chemistry of our college.

I would like to gratefully acknowledge the support extended by the Assam Science Society in holding the conference.

(Dr. Satyendra Nath Barman)

Principal

B Borooah College

Guwahati, Assam, India.

From the Organiser's Desk

It is an honour and pleasure for us to welcome you all to the **International Conference on Progress and Challenges in Modern Day Science (PCMDS-2021)**, being organised by the Department of Chemistry, B. Borooah College in association with Assam Science Society on 17th and 18th June 2021.

Creativity and innovation are the catalyst of advancement. From time immemorial it has been recognised that education emancipates. However, no study is complete when the scope of further research is available. Research is the fuel for advancement and development. This conference provides a platform where researchers will contribute and present their views.

Francis Bacon said "Reading maketh a full man; conference a ready man; and writing an exact man". Conferences bring together people of varied experiences and provide an opportunity to everyone to share their thoughts. Mutual participation and high quality deliberations create an inspiring learning environment resulting in innovative ideas.

We hope that the conference will be a wonderful opportunity for the participants to gain quality input useful for their future research in this knowledge based society.

We are indeed pleased to state that in this conference we have one session specifically dedicated to women scientists in honour of Dr Sutopa Raichaudhury, Head of the Department of Chemistry of our College, who is retiring on 30th June 2021. She has been serving the department for over 35 years and has been instrumental in shaping the lives of many students.

We are extremely grateful to the Assam Science Society for their kind support in organising this conference. We take this opportunity to express our gratitude to the principal of our college for helping us in every aspect of the conference.

The conference is being organised in the virtual mode with Zoom platform being used for oral sessions and Twitter and Facebook for the poster sessions. We do acknowledge the importance and relevance of these platforms because of which we have been able to hold the conference at these troubling times of Covid-19.

Team PCMDS-2021

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Sl. No.	Author	Title
	Prof. Pratap Jyoti Handique	Key Note Address
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IL-2	Dr. Rupam Jyoti Sarma	Design and Development of Anthracene-derived Mechano-Luminescent Solids
IL-3	Dr. Pankaj Kumar Koli	Nitric Oxide to Various Species: Finding the New Mechanistic Insights of Enzyme Mimics
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**International Conference
On
Progress and Challenges in Modern Day Science (PCMDS-2021)**

Date: 17th & 18th June, 2021

Programme Schedule

Day 1		17th June
Inaugural Session		
09.00 - 09.25	Joining the Conference on Zoom	
09.25 - 09.30	Introductory remarks by convener	
09.30 - 09.35	Welcome address Dr. Satyendra Nath Barman <i>President, PCMDS-2021 & Principal, B. Borooah College, Assam, India</i>	
09.35 - 09.40	Opening Remarks Prof. Mohan Ch. Kalita <i>President, Assam Science Society, Assam, India</i>	
09.40 - 10.10	Key Note Address Prof. Pratap Jyoti Handique <i>Vice Chancellor, Gauhati University, Assam, India</i>	
10.10 - 10.15	Vote of thanks	
Break (40 minute)		
Session I		
10.55 - 11.00	Chair: Prof. Dibakar Chandra Deka <i>Honourable Vice Chancellor, Madhabdev University, Assam, India</i>	
11.00 - 11.55	PL-1: Prof. Thalappil Pradeep <i>Department of Chemistry, IIT Madras, India</i>	
11.55 - 12.25	IL1: Dr. Mausam Kalita <i>Stanford University, USA</i>	
Break (30 minute)		
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13.00 - 13.30	IL 2: Dr. Rupam Jyoti Sarma <i>Department of Chemistry, Gauhati University Assam, India</i>	IL 3: Dr. Pankaj Kumar Koli <i>Department of Chemistry, IISER Tirupati, India</i>
13.30 - 13.45	SIL 1: Dr. Bidyut Bikash Sarma <i>Department of Chemistry, Karlsruhe Institute of Technology, Germany</i>	SIL 3: Dr. Hemanta Deka <i>Schulich Faculty of Chemistry, Technion-Israel Institute of Technology, Israel</i>
13.45 - 14.00	SIL 2: Dr. Pulakesh Das <i>Department of Chemistry and Biochemistry, Rowan University, USA</i>	SIL 4: Dr. Biswajit Sahariah <i>New Chemistry Unit, JNCASR, India</i>
14.00 - 14.10	OP 1: Debojit Paul <i>Department of Chemistry, IIT Guwahati</i>	OP 6: Sudip Shit <i>Department of Chemistry, IIT Guwahati</i>
14.10 - 14.20	OP 2: Kalpita Baruah <i>Department of Chemistry, Shiv Nadar University, Noida, India</i>	OP 7: Sourav Bhowmick <i>Department of Chemistry, IIT Guwahati</i>
14.20 - 14.30	OP 3: Debajyoti Debnath <i>Department of Chemistry, Presidency University, Kolkata, India</i>	OP 8: Shilpika Khanikar <i>Assam Donbosco University, India</i>
14.30 - 14.40	OP 4: Lakhya Jyoti Mazumder <i>Cotton University, Assam, India</i>	OP 9: Ritesh Kant Gupta <i>Department of Chemistry, IIT Guwahati</i>

14.40 - 14.50	OP 5: Samiran Upadhyaya <i>Institute of Advanced Study in Science and Technology (IASST), India</i>	OP 10: Pranjal Saikia <i>Nowgong College, Assam, India</i>
Break (35 minute)		
Session IV		
15.25 - 15.30	Chair: Dr. Tridib Kumar Sarma <i>Department of Chemistry, IIT Indore</i>	
15.30 - 16.25	PL-2: Prof. Tomislav Friscic <i>Department of Chemistry, McGill University, Montreal, Canada</i>	
16.25 - 16.55	IL 4: Dr. Gabriela Schneider Rauber <i>Postgraduate Programme of Pharmacy, Federal University of Santa Catarina, Brazil</i>	
16.55 - 17.25	IL 5: Dr. Rupam Sarma <i>Department of Chemistry, University of Kentucky, USA</i>	
17.25 - 17.40	SIL 5: Dr. Abdur Rahim <i>The State University of New York at Buffalo (SUNY Buffalo), Buffalo, USA</i>	
End of Day 1		
Day 2		18th June
08.30 - 08.55	Joining the Conference on Zoom	
Session V <i>(Women Scientists Session in Honor of Dr Sutopa Raichaudhury, Head, Department of Chemistry, B. Borooah College, Assam, India)</i> <i>(Dr Sutopa Raichaudhury is going to retire on 30th June, 2021 after more than three decades of service)</i>		
08.55 - 09.00	Chair: Prof. Upasana Bora Sinha <i>Dept. of Chemistry, Nagaland University, India</i>	
09.00 - 09.30	IL 6: Dr. Geetha Bolla <i>Department of Chemistry, Bengurion University, Israel</i>	
09.30 - 09.45	SIL 6: Dr. Sudesna Chakravarty <i>Virginia Commonwealth University, USA</i>	
09.45 - 10.00	SIL 7: Dr. Tarali Devi <i>Department of Chemistry, Humboldt-Universität zu Berlin, Germany</i>	
10.00 - 10.15	SIL 8: Dr. Gargi Buragohain <i>Department of Chemistry, Cotton University, Assam, India</i>	
10.15 - 10.25	OP 11: Kangkana Deka <i>Department of Chemistry, Gauhati University, Assam, India</i>	
10.25 - 10.35	OP 12: Bhupalee Kalita <i>Department of Chemistry, University of California, USA</i>	
10.35 - 10.45	OP 13 : Biva Talukdar <i>National Yang Ming Chiao Tung University, Taiwan</i>	
10.45 - 10.55	OP 14: Hemrupa Kuilya <i>Department of Chemistry, B. Borooah College, Assam, India</i>	
10.55 - 11.05	OP 15: Munmi Sarma <i>Department of Chemistry, UniversitatAutonoma de Barcelona, Spain</i>	
Break (40 Minute)		
	Session VI	Session VII
11.45 - 11.50	Chair: Dr. Pranjit Barman <i>Department of Chemistry, NIT Silchar</i>	Chair: Dr. Rupam Jyoti Sarma <i>Department of Chemistry, Gauhati University, Assam, India</i>
11.50 - 12.20	IL 7: Dr. Bipul Sarma <i>Department of Chemical Sciences, Tezpur University, Assam, India</i>	IL 8: Dr. Ankur K Guha <i>Department of Chemistry, Cotton University, Assam, India</i>
12.20 - 12.35	SIL 9: Dr. Biju Majumdar	SIL 13: Dr. Asif Ansari

	<i>Department of Chemistry, University of California, USA</i>	<i>Institute of Inorganic Chemistry, University of Gottingen, Germany</i>
12.35 - 12.50	SIL 10: Dr. Najrul Hussain <i>Center for Advanced Materials Research, University of Sharjah, UAE</i>	SIL 14: Dr. Arijit Singha Hazari <i>Institut für Anorganische Chemie, Universität Stuttgart, Germany</i>
12.50 - 13.05	SIL 11: Dr. Monoj Mon Kalita <i>Senior Regulatory Affairs Specialist, Unimax Medical Systems Inc., Taiwan</i>	SIL 15: Dr. Aswini Kalita <i>Department of Chemistry, Sipajhar College, Assam, India</i>
13.05 - 13.20	SIL 12: Dr. Jyotirmoy Sarma <i>Department of Chemistry, Kaziranga university, Assam, India</i>	SIL 16: Dr. Rajesh Deka <i>Department of Chemistry Uppsala University, Sweden</i>
13.20 - 13.30	OP 16: Dr. Chandan Sharma <i>Morigaon College, Assam, India</i>	OP 22: Mousumi Baruah <i>Department of Chemistry, Shiv Nadar University, Noida, India</i>
13.30 - 13.40	OP 17: Nikita Chakraborty <i>Department of Chemistry, IIT Guwahati</i>	OP 23: Subhamoy Biswas <i>Department of Chemistry, IIT Guwahati</i>
13.40 – 13.50	OP 18: Amar Ghosh <i>Behala College, Calcutta University, Kolkata, India</i>	OP 24: Pankaj Saikia <i>Tinsukia College, Assam, India</i>
13.50 – 14.00	OP 19: Rabindranath Garai <i>Department of Chemistry, IIT Guwahati</i>	OP 25: Dr. Biswajit Deb Roy <i>Cachar College, Silchar, Assam, India</i>
14.00 – 14.10	OP 20: Hiranya Gogoi <i>Department of Chemistry, IIT Guwahati</i>	OP 26: Tamanna Khandelia <i>Department of Chemistry, IIT Guwahati</i>
14.10 – 14.20	OP 21: Dr. Nijan Chandra Pegu <i>B. Borooh College, Assam, India</i>	OP 27: Dr. Dhanjit Deka <i>Gauhati University, Assam, India</i>
Break (35 Minute)		
Session VIII		
14.55 - 15.00	Chair: Prof. Pranab Jyoti Das <i>Retd. Professor, Dept. of Chemistry, Gauhati University, Assam, India</i>	
15.00 - 15.55	PL 3: Prof. William Jones <i>Department of Chemistry, University of Cambridge, UK</i>	
15.55 - 16.25	IL 9: Dr. Debajit Sarma <i>Department of Chemistry, IIT Patna</i>	
16.25 – 16.40	SIL 17: Dr. Partha Jyoti Das <i>Department of Chemistry, Northwestern University, USA</i>	
16.40 – 16.55	SIL 18: Dr. Diganta Kalita <i>Research Chemist, Van Drunen Farm, FutureCeuticals Inc., USA</i>	
Valedictory Session		
17.00 – 17.05	Address by Dr. Jagadindra Raichoudhury , <i>Secretary, Assam Science Society, Assam, India</i>	
17.05 – 17.10	Declaration of Best Poster Award	
17.10 – 17.15	Closing remarks by Dr. Satyendra Nath Barman , <i>Principal, B. Borooh College, Assam, India</i>	
17.15 – 17.20	Closing remarks by Dr. Sutopa Raichaudhury , <i>Head, Department of Chemistry, B. Borooh College, Assam, India</i>	
17.20 – 17.25	Vote of thanks	

(PL: Plenary Lecture; IL: Invited Lecture; SIL: Short Invited Lecture; OP: Oral Presentation)

Timing of Poster Presentation

- Online Poster Presentation will be held simultaneously on the Face book page (**Pcmds-2021**) and Twitter (@Pcmdschembbc).
- Poster session will start on Wednesday, June 16 at 10:00 a.m. IST and will continue till the end of the conference.
- Poster presenters are requested to pin their poster tweet to @Pcmdschembbc before the start of the Poster session (Wednesday, June 16 at 10:00 a.m.). Participants are also requested to upload their poster on the face book page 'Pcmds-2021' as an image (JPEG format) with standard poster dimensions by creating a post.

Keynote address

Progress and Challenges in Modern Science

Prof. Pratap Jyoti Handique

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This discussion is mostly a review based comments on progress and challenges in science. An attempt has been made to identify the nature and process of progress in science. Various discussions and comments on historical and philosophical perspective have been analyzed to qualify and interpret scientific progress. Well accepted concept on challenges facing by science has also been presented.

Assessing the progress in science is an intricate philosophical and empirical procedure. It is evident that progress generally indicates moving forward in a positive way. A number of theories and experimental findings have been developed on the overlapping theme of progress in science and the aspects that contribute to scientific discoveries. Though we witnessed the extent of scientific advancement and utilized the benefit of scientific products, but assessing the progress in science is a complicated task. It requires combined historical, philosophical and sociological deliberations.

It is a well-known perception that modern science is a process of understanding the natural and physical world, based on recognizable evidence or proof, interpretation, and repeated testing. Various schools of thought opined that the process in the scientific method involves making hypotheses, deriving prediction or calculation from them as logical consequences, and then carrying out experiments or empirical observations based on those predictions. These hypotheses are then tested by scientists conducting experiments or other form of studies. The modern science has been growing and progressing for last about 500 years since the days of Galileo within these basic philosophical framework and practices. It is worth mentioning that Albert Einstein called Galileo the “father of modern science.” Until the time of Galileo Galilei, the Earth was thought to be the center of the universe. Galileo's mathematics based objective observations has changed this perception and ignited one of the foundations of modern science. However, according to several historical notes the earliest dates for the birth of modern science range from the High Middle Ages in 1277 through the 17th century. Some historians cite a second scientific revolution to have occurred in the early 20th century with the advent of quantum physics.

“A Strategy for Assessing Science” (A National Academies Press (US) publication, 2007) stated that “science makes progress when it develops concepts, typologies, frameworks of understanding, methods, techniques, or data that make it possible to uncover phenomena or test explanations of them. Thus, knowing where and how to look for discoveries and explanations is an important type of scientific progress. The history of science has produced several general theories about how science develops and evolves over long periods of time. A 19th century view is that of Auguste Comte, who argued that there is a hierarchy of the sciences, from the most general (astronomy), followed historically and in other ways by physics, chemistry, biology, and sociology. Sciences atop the hierarchy are characterized as having more highly developed theories; larger use of mathematical language to express ideas; higher levels of consensus on theory, methods, and the significance of problems and contributions to the field; more use of theory to make verifiable predictions; faster obsolescence of research, to which citations drop off rapidly over time; and relatively fast progress. Sciences at the bottom of the hierarchy are said to exhibit the opposite characteristics” (Cole, 1983)^[1].

The above compilation also discussed various types of scientific progress that included – the discoveries of phenomena, theoretical explanations or syntheses, tests of theories or hypotheses, acceptance or rejection of hypotheses or theories by the relevant scientific communities, development of new measurement or analytic techniques, application of general theory to specific theoretical or practical problems, development of technologies or useful interventions to improve human health and well-being from scientific efforts, and so forth. Consequently, many different developments might be taken as indicators, or measures, of progress in science.

A recent study on scientific progress has described “Science as a multi-layered complex system involving a community of scientists engaged in research using scientific methods in order to produce new knowledge. Thus, the notion of science may refer to a social institution, the researchers, the research process, the method of inquiry, and scientific knowledge. The concept of progress can be defined relative to each of these aspects of science. Hence, different types of progress can be distinguished relative to science: *economical* (the increased funding of scientific research), *professional* (the rising status of the scientists and their academic institutions in the society), *educational* (the increased skill and expertise of the scientists), *methodical* (the invention of new methods of research, the refinement of scientific instruments), and *cognitive* (increase or advancement of scientific knowledge)” [2].

Progress in science is a successive process and it involves making hypotheses, deriving predictions from them as logical consequences, and then carrying out experiments based on those predictions to determine whether the original hypothesis was correct. The basic elements of the scientific method can be illustrated by the discovery of the structure of DNA where all the above mentioned steps of the process were involved [3].

However, science has been facing various challenges in performance, application and progress. According to a survey based story, seven biggest challenges are faced by science. These are - huge money problem in academia, numerous poorly designed study, replicating result is crucial and rare, peer review are broken, too much science is locked behind pay walls, science is poorly communicated, and, life as a young academic is extremely stressful^[4]. Omenn (2016) has identified the grand challenges in specific fields of science like mathematics, physics and astronomy, environmental sciences, genetics and genomics, proteomics, systems biology and drug development, and various other multidisciplinary R&D areas [5]. He also identified the role of science and technology to help address societal risks. In the present Covid-19 emergency it is very pertinent to discuss the role of science in solving these problems.

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Molecular chemistry of nanoparticles

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Research in the recent past has resulted in a large number of nanoparticles whose properties depend on the number and spatial arrangement of their constituent atoms. This distinct atom-dependence of properties is particularly noticeable in ligand protected atomically precise clusters of noble metals. They behave indeed like molecules as revealed most elegantly by mass spectrometry. They show unusual properties such as luminescence in the visible and near-infrared regions. Their molecule-like behavior is most elegantly shown by atom and structure conserving chemical reactions between them. Several clusters, which are archetypal nanoparticles, $\text{Ag}_{25}(\text{SR})_{18}$ and $\text{Au}_{25}(\text{SR})_{18}$ (-SR = alkyl/aryl thiolate) have been used for such reactions. Despite their geometric robustness and electronic stability, reactions between them in solution at room temperature produce alloys $\text{Ag}_m\text{Au}_n(\text{SR})_{18}$ ($m+n = 25$), keeping their $\text{M}_{25}(\text{SR})_{18}$ composition, structure and topology intact. We captured one of the earliest events of the process, namely the formation of the dianionic adduct, $[\text{Ag}_{25}\text{Au}_{25}(\text{SR})_{36}]^{2-}$, by electrospray ionization mass spectrometry.

Exploring this science further, we have studied rapid solution state exchange dynamics in nanoscale pieces of matter, taking isotopically pure atomically precise clusters as examples. As two isotopically pure silver clusters made of ^{107}Ag and ^{109}Ag are mixed, an isotopically mixed cluster of the same entity is formed, similar to the formation of HDO, from H_2O and D_2O . This spontaneous process is driven by the entropy of mixing and involves events at multiple timescales.

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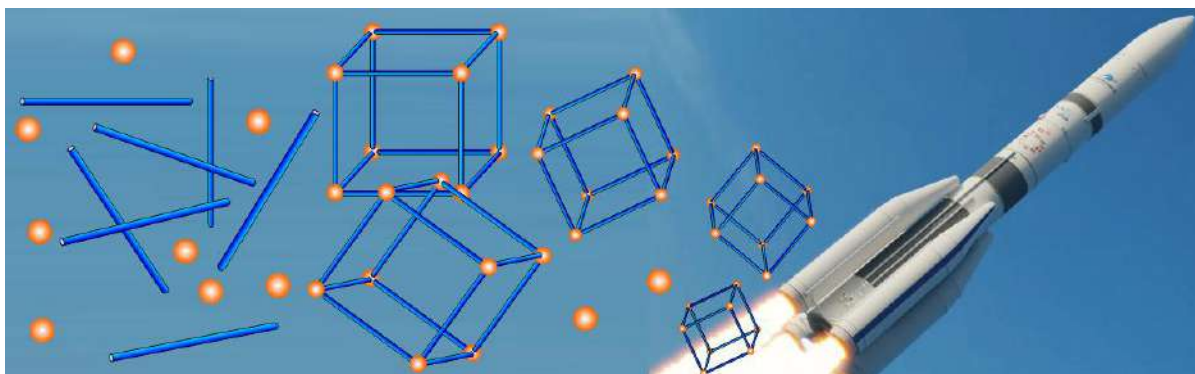
Directing the (in)stability of metal-organic frameworks (MOFs)

Prof. Tomislav Friščić

Department of Chemistry, McGill University

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This presentation will outline our recent contributions in using experimental and theoretical methodologies to understand and even predict the thermodynamic stability of metal-organic frameworks (MOFs).^{1,2}



In particular, we will highlight the potential for the development of simple guidelines to design MOFs with controllable stability based on established or readily accessible descriptors of molecular stability,³ and describe the use of this class of materials as a foundation for the development of a new type of greener and tuneable aerospace fuels⁴ – whose ignition and energy output could be controlled through molecular-level design and crystal engineering.

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PL-3

Disappearing polymorphs

Prof. William Jones

Yusuf Hamied Department of Chemistry, University of Cambridge, UK

In this talk I will briefly introduce pharmaceutical solids for the delivery of drug molecules and touch upon the concept of polymorphs and how polymorph variations can affect the manufacture and effectiveness of a formulation. I will then introduce mechanochemistry as a technique for exploring solid form diversity and especially the ability of mechanochemistry to screen for various solid forms. The final section will introduce the concept of “disappearing polymorphs” when it appears that a previously well-established crystal form can no longer be made even though efforts are made to reproduce as precisely as possible previous experimental protocols.

Biomedical Imaging Toolbox: Nanosensors and PET Tracers

Dr. Mausam Kalita

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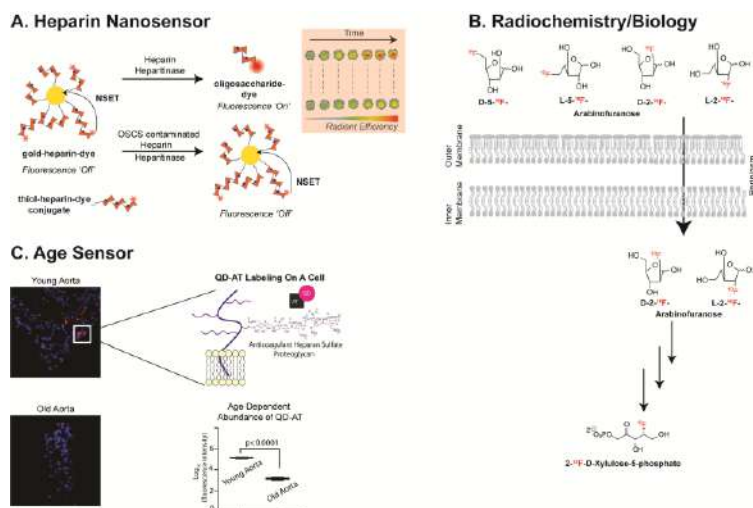


Figure. A) gold-heparin-dye nanosensor detects contaminants (over-sulfated chondroitin sulfates) in the pharmaceutical grade heparin with limit of detection of 10^{-9} % (w/w) (*J. Am. Chem. Soc.* 2014, 136(2): 554-557), B) A library of arabinofuranose-derived ^{18}F PET radiotracers was synthesized with high radiochemical purity. Both D-2- ^{18}F -AF and L-2- ^{18}F -AF showed sensitivity to most gram-negative and gram-positive organisms (*J Labelled Comp Radiopharm.* 2020, 63(5): 231-239), C) The quantum dot-antithrombin III (QD-AT) probe detects rare 3-*O*-sulfated heparan sulfate structures. The high-resolution images reveal abundant AT-binding structures in the blood vessels of a two weeks old mouse aorta. In contrast, there is a significant decrease in anticoagulant active structures in a six months old mouse aorta (*Chemical Communications*, 2020, 56(92): 14423-14426).

Modern science has revolutionized human health research. The rapid pace of diagnosis and treatment of human diseases involves a scientific ecosystem of chemistry, biology, and technology (mathematics and instrumentation). In the labs at the University of California and Stanford Hospitals, we focus on developing diagnostic and therapeutic solutions for cancer, neurodegenerative disorders, and infectious diseases. In this seminar, I will focus on our recent state-of-the-art imaging tools based on glycoscience. We constructed a gold-heparin-dye nanosensor to identify over-sulfated chondroitin sulfates (OSCS) contaminant in the pharmaceutical grade heparin, a life-saving drug. This technology can aid the regulatory bodies to detect this life-threatening contaminant in life-saving heparin. Next, we leveraged the bacterial metabolic program to develop diagnostic PET tracers. The 2- ^{18}F -D- and L- arabinofuranoses avidly incorporate into both gram-negative and gram-positive bacteria. Therefore, these probes can potentially be used as PET tracers to diagnose a broad range of bacterial infections. Finally, to map structurally diverse heparan sulfate (HS) epitopes, we conjugated quantum dot (QD) with antithrombin III (AT) and FGF2 proteins to generate QD-AT and QD-FGF2 probes. These two probes revealed abundance and distribution of rare, anticoagulant 3-*O*-sulfated pentasaccharide and ubiquitous 2-*O*-sulfated tetrasaccharide motifs of HS in endothelial cells and aortic tissue sections with excellent resolution. Our study demonstrated the utility of QD-AT (and QD-FGF2) in identifying age-associated changes in HS motifs. The technology for rare HS motifs might pinpoint the risk factors such as age-associated thrombosis and neurodegeneration.

Design and Development of Anthracene-derived Mechano-Luminescent Solids

Dr. Rupam Jyoti Sarma

Department of Chemistry, Gauhati University

Mechano-luminescence (ML) refers to a unique property by which certain materials emit light (or become emissive) upon application of mechanical force or stimulus.^{1,2} Studies have revealed that the emission color of ML materials could extend over a broad spectral range, from ultraviolet to visible and infrared light. In this context, the design and synthesis of organic luminogens that produce bright emissions in the solid state in response to mechanical stimuli have attracted immense attention, in view of their potential applications as deformation detectors, sensors and optoelectronic devices.³

Our investigations have shown that the anthracene moiety can serve as a versatile building block for the development of organic ML materials. While a detailed understanding of the origins of ML activity in such molecular solids remains obscure, the role of molecular structure, packing arrangements and intermolecular interactions has been highlighted.^{4,5} For instance, reversible switching between polymorphic forms of anthracene-derived luminogens could be achieved using mechanical stimuli, and thermal stimuli.⁶ However, the observation of ML activity in organic solids seems relatively rare, and in most instances, changes molecular orientations or intermolecular interactions are quite difficult to predict.⁷

The search for generalized understanding of the conditions under which organic solids can become ML active requires detailed understanding of (i) molecule-crystal, and (ii) crystal-property relationships.⁷ In this context, characterizing the polymorphic forms of the organic luminogen offer a reliable approach towards deciphering how mechanical stimuli (viz. pressure, compression, friction) can induce subtle changes in the solid state structures, i.e. molecular geometry, packing arrangements and intermolecular interactions.^{7,8} By doing so, we hope to identify suitably functionalized anthracene derivatives capable of exhibiting mechano-luminescent and thermochromic behavior in the solid state.

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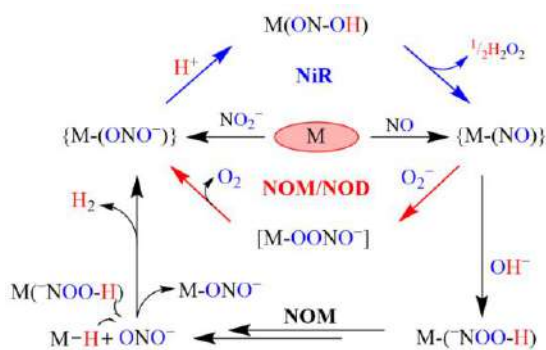
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Nitric Oxide to Various Species: Finding the New Mechanistic Insights of Enzyme Mimics

Dr. Pankaj Kumar Koli

Indian Institute of Science Education and Research Tirupati

Nitric oxide (NO) attracted enormous interest from chemists and biochemists due to its significant effect on the biological system. For instance, NO is widely known as a signal transduction molecule for the involvement in major biological processes, such as neurotransmission, vascular regulation, platelet disaggregation, and immune response to bacterial infections.¹ In this regard, nitric oxide synthases (NOSs) and Nitrite reductases (NiRs) accomplished the constant NO biosynthesis. NiRscatalyze the production of NO by nitrite (NO_2^-) reduction in the presence of protons, i.e., $\text{NO}_2^- + e^- + 2\text{H}^+ \rightarrow \text{NO} + \text{H}_2\text{O}$. However, when produced in a higher amount, it stimulates the reactive nitrogen species (RNS) and causes carcinogenesis and neurodegenerative disorders.² Microbial and mammalian systems have a unique mechanism to convert the excess NO to biologically benign nitrate (NO_3^-) by using nitric oxide dioxygenase (NODs) enzymes. The interesting fact is in both the NiR and NOD reactions, heme-containing Fe moiety is involved. Apart from this, NO-releasing molecule sodium nitroprusside (NP) undergo nitric oxide monooxygenation (NOM) reaction to generate NO_2^- under primary conditions. Thus, one metal is involved in converting NO to NO_2^- and NO_3^- and vice versa. Our motivation to mimic all the reactions in one metal complex in vivo system leads us to develop a Co complex bearing 12TMC ligand framework $[(12\text{-TMC})\text{Co}^{\text{II}}]^{2+}$ complex. Interesting facts about this complex show dioxygen activation, NO activation, NOD reactivity,³ NiR reactivity⁴, and NOM reactivity⁵. Apart from this versatile character of this complex and higher stability of its metal-NO complex, it also exhibits NO transfer reaction in the presence of a suitable acceptor. This multipurpose reactivity of a single molecule helps us study all the reactions mentioned above in a single metal complex and understand their dependence on the metal center and the ligand framework.



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TITLE: “I made a book, but I have not lost the poetry”

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A few years ago, I had just finished my master’s and was invited to my first Viva as an examiner. Of the many things I have learnt on that day, I recall a comment another examiner made after the student and I finished our conversation. He said that by listening to us he remembered his younger self. In the talk today I invite you to remember and honour both inner aspects of yours, the curious cheerful student and the wise resilient supervisor. As a background to your memories, I will share a glimpse of the progress and challenges I have been experiencing as a scientist working with solid-state chemistry of pharmaceuticals. Carbamazepine will be used as an example to explore aspects considered in the selection of crystal forms for drug delivery, especially bulk and surface characteristics, particle breakage and phase transformations.^{1,2}

The title of the talk refers to a poem by Adélia Prado called “Fluency”(1977)

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Bio-inspired Membranes: Application Towards Pollutant Degradation and Value-Added Transformation

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Bio-inspired membrane with immobilized enzymes on it provides versatile platforms for applications ranging from environmental remediation to generation of value-added chemicals from waste. Despite associated environmental concerns, the existing techniques for remediating pollutants in water consist of both physical and chemical means mostly using heavy metals. To offer bioremediation as an alternative option, we herein demonstrate a layer-by-layer approach to immobilize enzyme into functionalized membranes. This mode of membrane functionalization provides a synergistic platform for pollutant degradation where leaching of heavy metals into the environment is unacceptable. The enzyme-functionalized membrane was characterized by a wide variety of spectroscopic and microscopic techniques including ATR FT-IR, SEM imaging and XPS analysis and more. The stability of the enzyme in both solution phase and on membrane phase was studied. Enzyme showed a loss of some 65% of initial activity in the solution phase after weeks of use, whereas the membrane-bound enzyme lost only a negligible percentage of activity in the same time span. Activity of these biomimetic membranes towards dechlorination of 2,4,6-trichlorophenol (TCP) is demonstrated under pressure driven continuous flow mode. Up to 80% of the initial TCP was degraded at optimum flow rate. The membrane was exposed to rigorous cycles of TCP exposure to study its long term activity and reusability. The primary results reveal that our laccase-functionalized membrane lost only 14% of its initial activity in a period of 25 days. Finally, the reusability of the membrane as a support material was also demonstrated by detaching and re-immobilizing the enzyme on the membrane-polymer domain for multiple consecutive cycles.

We have further extended the layer-by-layer approach to fabricate multienzyme functionalized membrane reactor for bioconversion of lignin model compound involving enzymatic reactions. Three different enzymes (glucose oxidase, peroxidase and laccase) were immobilized into functionalized PVDF membranes. This novel membrane reactor couples the in-situ generation of hydrogen peroxide to oxidative conversion of a lignin model compound, guaiacylglycerol-B-guaiacylether (GGE). Preliminary investigation of the efficacy of these functional membranes towards GGE degradation is demonstrated under convective flow mode. Over 90% of the initial feed could be degraded with the multienzyme immobilized membranes. GGE conversion product analysis revealed formation of oligomeric oxidation products with peroxidase, which might be potential hazard to membrane bioreactors. These oxidation products could be further degraded by laccase enzymes in the multienzymatic membranes explaining the potential of multienzyme membrane reactors.

I acknowledge the support from University of Kentucky and NSF-EPSCoR program for carrying out this research.

Preparation of Crystalline Smart Materials along with design and Organic Biomineralization

Dr. Geetha Bolla

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My research is to focus and investigation of the

- Organic biomineralization, chromatophore cells, organic bioinspired optical materials crystallization mechanisms. Biogenic crystals.
- Heterogeneous nucleation, SURMOFs design, polymorphs, cocrystals of the pharmaceutical drugs, organic optoelectronics, waveguides. Organic cocrystals and polymorphs.
- Structural aspects of novel multi-functional molecular actuator of the mechanosensitive metal complexes as smart material advanced applications. Photo and Thermosensitive complexes.

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Guiding Crystallization Events by Functional Monolayers/Organogels

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Crystallization process is an extremely important phenomenon.¹ But, these events can be guided at the interface of organic monolayers expressed by directional intermolecular interactions. Several organic thiols were introduced to prepare such functional self-assembled monolayers (SAMs) on gold surface to control the crystallization process of conformationally flexible drug molecules. Drug mefenamic acid and sulfathiazole, both are conformationally flexible and known for its concomitant crystallization were chosen as representative examples. The organic monolayers were identified as effective template to nucleate desired polymorphic phases of the drug.^{2,3} Another peer strategic approach to control the polymorphism of functional group related drugs by introducing a drug-mimetic functional group into organogels was also introduced. The urea based organogelators designed to form gels acted as template to control concomitant crystallization of mimetic drugs like (\pm)-thalidomide and barbital.⁴ These two approaches established the potential to control the crystallization events, a serious issue in the drug formulation department.

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IL-8

In silico study of some non-classical compounds of main group elements

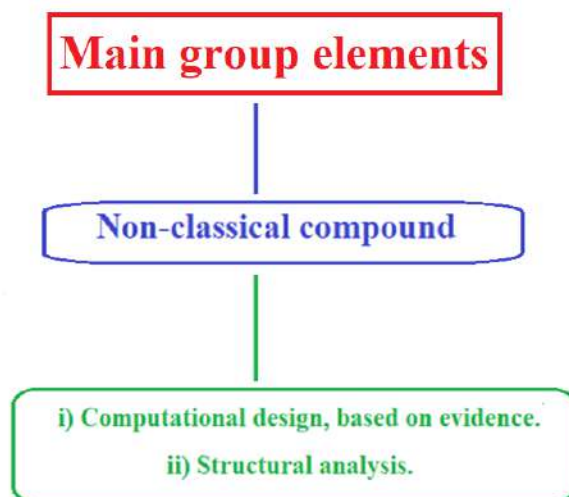
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Non-classical main group compounds are an interesting class of compounds owing to their unconventional structural features. Among the contemporary non-classical compounds of main group elements, planar hypercoordinate clusters have gained popularity among the chemists. One of the key features of these compounds is the presence of multifold aromaticity which attribute to their high stability. Computational chemistry plays an important role in identifying different planar hypercoordinate clusters by searching the potential energy surface for possible identification of different minimas. Likewise planar hypercoördinte clusters, quadruple bonding in main group elements is also a challenging task. This is because of the unavailability of d-electrons. But if we can incorporate a transition metal with main group element, then we may achieve this feat as the transition metal or its fragment will play the major role by using its available d-electrons for eastablishing the four fold bonding. With the advancement in spectroscopic techniques, both the planar hypercoordinate clusters and quadruple bonded compounds of main group elements are being realized at the experimental level. High level theoretical studies for such compounds is important to understand the electronic feature at the quantum level.

Keywords: Non-classical structure; main group elements; *ab initio* study.



Functional Metallogel and Framework Materials for Environmental Remediation and Related Applications

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Heavy industrialization in search of a better human life is adversely affecting quality of available clean water, which is central to sustain human civilization on this planet. Heavy metal ions (Cd^{2+} , Hg^{2+} , As^{3+} and Pb^{2+}), various oxoanions ($\text{Cr}_2\text{O}_7^{2-}$, CrO_4^{2-} etc.), spent nuclear fuels (^{90}Sr , ^{137}Cs , and ^{127}I) and soluble organic dyes are the main contributor for the contamination of the water bodies. The selective removal of these ions/molecules are of utmost importance. Herein, we report the development of various functional sulfide based ion exchangers, for ion exchange of soft metal ions and oxoanions. Layered materials,¹ supertetrahedral framework² and metal organic framework based composites³ exhibits excellent ion exchange properties in varying conditions. Facile metallogel materials are also developed for adsorption and separation of water soluble dyes.^{4,5} Some of these materials are also found to extract water from the atmospheric moisture with three-fold adsorption capacity by their weight. These tunable metallogels can also be used for other applications such as near-white light-emission by careful incorporation and stoichiometric control of Tb^{III} : Eu^{III} ions. The facile synthesis of these framework and metallogel materials coupled with its excellent sorbent properties underscores its potential in environmental remediation and other related applications.

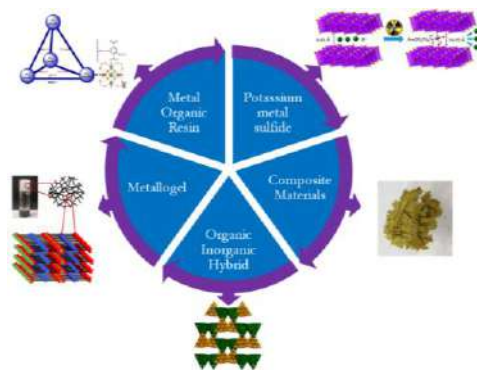


Figure 1. Schematics of Functional Metallogels and Framework Materials for Environmental Remediation

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Supported Single Atom Catalysts: Understanding the Dynamics of Active Center under Operando Conditions

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An exciting ongoing interest in heterogeneous catalysis is understanding the behavior of atoms anchored over support, which is often referred to as single-atom catalysts (SACs).^[1] Single atom can be anchored over various supports such as metal-oxide, 2D carbon like materials, 3D materials such as zeolite, metal-organic framework and in the host matrix of other array of atoms. When stabilized over these materials, single atom exhibits different degree of coordination, charge on the metal and confinement within the support. These parameters firmly determine the driving force with regard to catalyst stability, performance towards catalytic reactions and frequently governs the selectivity of the products. However, identifying single atom over support is a challenge since most of the laboratory available techniques have certain barriers. Hence, synchrotron-radiation based X-ray absorption spectroscopy (XAS) is seen as one of the emerging techniques in this area of research. XAS can be applied across the periodic table to identify oxidation state of metals, bond distances between the neighbour and symmetry around the active center, even under operating conditions, upto a bond distance of 5-6 Å.

Moreover, as already established, solid catalysts are often less flexible and the active sites may be unevenly distributed. In order to understand the dynamic nature of solid catalysts, breaking down the solid catalyst to single atom or to atomically dispersed species provides a great opportunity. In our work, we have shown with the help of X-ray absorption spectroscopy (XAS), aberration corrected high angle annular dark field scanning transmission electron microscopy (C_s -HAADF STEM), Fourier transform infrared (FTIR) spectroscopy with probe molecules like CO at low temperature whether the active species are either single atoms, clusters or nanoparticles.^{[2]-[3]} After thorough understanding of these techniques, further questions rise (a) Can supported single atom catalysts be a universal model for understanding every reactions? (b) How dynamic is the active center? and (c) What is the role of dynamic behavior of solid catalyst towards activity and selectivity during chemical reactions?

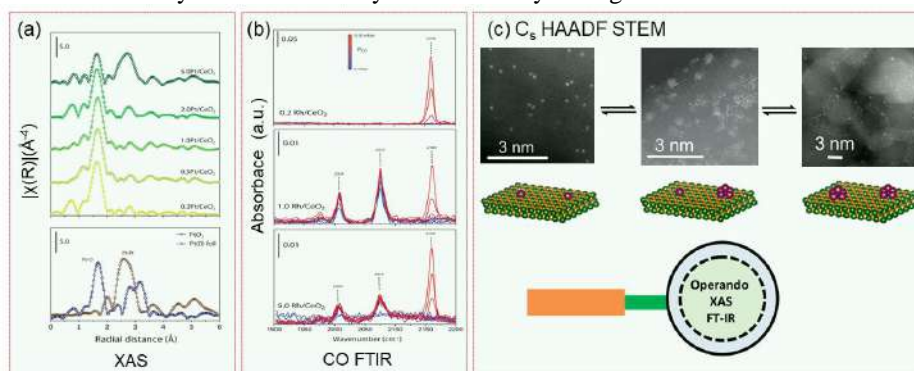


Figure 1. (a) XAS, (b) CO FTIR at liquid N_2 temperature and (c) C_s -HAADF STEM images of supported single atom, clusters and nanoparticle.

All these questions can be answered once we are very convinced about whether single atoms remain in its form under the truly operating reaction conditions. In our group at Karlsruhe Institute of Technology (KIT), directed by Prof. Jan-Dierk Grunwaldt, we are dedicated to designing special cells combining with different spectroscopic techniques where many more of industrially relevant reactions both in batch and in gas phase can be studied under operando conditions (*viz.* *operando* spectroscopy).

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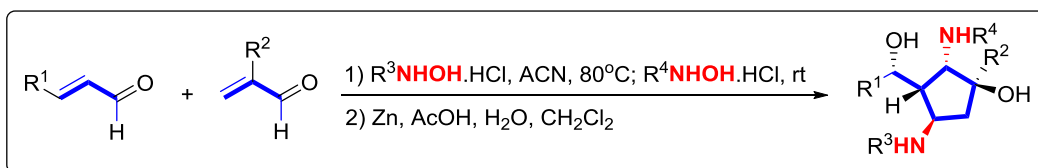
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Synthesis of Carbocyclic Nucleoside Analogues from Simple Enals and Hydroxylamines via Formation of Heterocycle

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Synthesis of substituted and stereochemically dense carbocycles can be achieved by the sequential dipolar cycloaddition followed by the reductive cleavage of vinylnitrones and enals. The reaction sequence proceeds effectively for a wide variety of enals and hydroxylamines. The reaction is regioselective as well as diastereoselective for the initial formation of a bridged-bisoxazolidine intermediate, which then endures quantitative double *N-O* bond cleavage to produce stereochemically dense carbocycles as a single diastereomer.



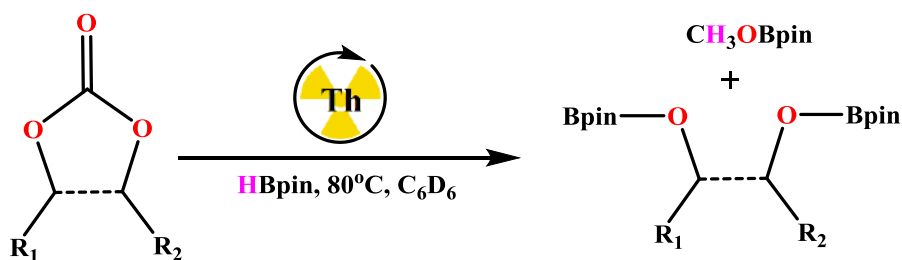
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Hydroboration of Organic Carbonate Catalyzed by Thorium Complexes of Iminato Ligand Hemanta Deka

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Three new thorium complexes of 5, 6, and 7 member *N*-heterocyclic iminato ligand with mesityl wingtip substitution have been synthesized. Increasing the core ring size ease the movement of the wingtip substitution in the complexes. Efficient reduction of cyclic and linear organic carbonates catalyzed by the prepared thorium complexes has been achieved. The described homogenous reaction provides an indirect route for the conversion of CO₂ into valuable alcohols. The reaction proceeds with high yields under mild reaction conditions, with low catalyst loading and short reaction times, and shows broad applicability toward various linear and cyclic carbonates. Additionally, the demanding depolymerization of polycarbonates achieved as well.



Spectroscopic evidence of $n \rightarrow \pi^*$ Interactions

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Noncovalent interactions are important in many chemical, biological and physical process and are abundant in both small- and macromolecules. Various types of weak noncovalent interactions including hydrogen bond, halogen bond, chalcogen bond, pnictogen bond, tetrel bond, carbon bond are widely studied. $n \rightarrow \pi^*$ interactions have gained a lot of attention among the chemist, biologist as well as material scientist in recent years.¹ When a lone pair of electrons (n) of a nucleophile is delocalized over the antibonding π -orbital (π^*) of an acceptor moiety, an overall stabilization of the system takes place. These stabilizing interactions are commonly known as “ $n \rightarrow \pi^*$ interaction”. Bürgi and Dunitz in the early 1970s identified short contacts between nucleophiles and carbonyl groups in high-resolution crystal structures of small molecules.² Their seminal work on $\text{Nu} \cdots \text{C}=\text{O}$ laid the foundation of the $n \rightarrow \pi^*$ interactions. Recent reports suggest that the relative orientation of carbonyl group determines the strength of $n \rightarrow \pi^*$ interaction.³ $n \rightarrow \pi^*$ interaction is relatively weak ($\sim 0.3\text{--}0.7 \text{ kcal}\cdot\text{mol}^{-1}$). The strongest $n \rightarrow \pi^*$ interaction could be as strong as a moderate hydrogen bond.⁴ Therefore, it is not straightforward to detect and quantify $n \rightarrow \pi^*$ interactions in solution and, naturally, spectroscopic investigations that can provide direct evidence of $n \rightarrow \pi^*$ interaction is limited. As the carbonyl group possess strong dipole moment, it is infrared active. As the carbonyl group accepts electron in the π^* orbital, the C=O bond order should decrease and, therefore, a red shift is expected in the C=O stretching frequency. Similarly, when a carbonyl group acts as a donor, there should be weakening of C=O bond strength and accordingly there should be a red shift in the C=O stretching frequency. Another spectroscopic method that may provide indication of $n \rightarrow \pi^*$ interaction is the ^{13}C NMR spectroscopy. In such instances, we provide computational support for the presence of $n \rightarrow \pi^*$ interactions by carrying out various computational studies including NBO, Atoms in Molecules (AIM) and Non-Covalent Interaction (NCI) analyses. We discuss spectroscopic evidence of $n \rightarrow \pi^*$ interaction in (i) solution (ii) gas-phase and (iii) N_2 and Ar matrices. Further, we also show that transannular interactions commonly observed in cyclic system are $n \rightarrow \pi^*$ in nature.⁵

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Solid-Phase Synthesis of Hybrid 2,5-Diketopiperazines Using Acylhydrazide, Carbazate, Semicarbazide, Amino Acid and Primary Amine Submonomers

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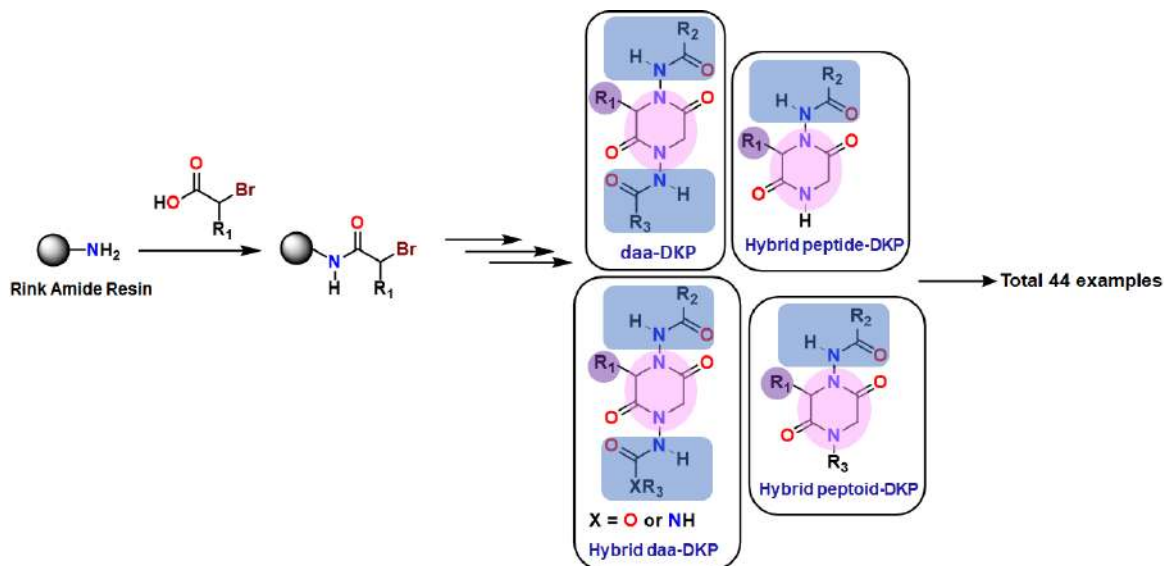
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Naturally occurring 2,5-DKP obey Lipinski rules and are widely used in drug discovery campaigns as they have many favourable properties including conformationally rigid, cell-permeability and proteolytic stability. Here, we report solid-phase synthesis of N,N'-di(acylamino)-2,5-diketopiperazine (daa-DKP), an acylhydrazide-based conformationally rigid 2,5-DKP scaffold having exocyclic N-N bonds. We also show that different combinations of acylhydrazides, carbazates, semicarbazides, amino acids and primary amines can be used to synthesize highly diverse collection of hybrid-DKP molecules via the solid-phase submonomer synthesis route. Finally, we show incorporation of a methyl substituent in one of the carbon atoms of the DKP ring to generate chiral daa- and hybrid-DKPs without compromising the synthetic efficiency.



Miniaturized *in vitro* Diagnostic Platforms for Cancer and Allied Diseases: Interplay of Chemistry, Engineering and Biomedical Sciences

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Smart miniaturized platforms constitute a major section of in vitro diagnostics (IVD). Herein, three types of miniaturized systems—miniaturised electrochemical platform, microfluidic integrated electrochemical platform and microfluidic integrated photothermal platform for cancer and allied diseases are discussed. Target biomarkers for the study include metabolites (glucose, ascorbic acid, cytokines), circulatory biomarkers (exosomes) and sialic acid respectively. The applicability of the miniaturized platforms are checked in clinical samples derived from healthy and diseased individuals (blood). They are found to be highly sensitive, selective and practical for real time sensing applications with a potential for monitoring of health conditions—Lung cancer, breast cancer and diabetes respectively.

Keywords: Microfluidics; Electrochemical; Photothermal; Miniaturized; Cancer; Diabetes

Tuning the Redox Reactivities of a Mononuclear Cr(III)-Superoxo Species by Proton and Lewis Acid Metal-Ions

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The metal-superoxo ($M^{n+}-O_2^{\cdot-}$) species have attracted much attention, since the intermediates have recently been invoked as reactive species in C-H bond activation of substrates in nonheme iron and copper enzymes.^[1] In respect to the chemical and biological redox reactions, it is also known that acid plays key roles in the proton-coupled electron-transfer (PCET) reactions such as the four-electron reduction of dioxygen in respiration and the four-electron oxidation of water by Mn_4CaO_5 cluster in the oxygen-evolving complex (OEC) in Photosystem II (PS II).^[2] Apart from proton, redox-inactive metal ions that act as Lewis acids also play as essential cofactors in modulating the redox reactivity of metal-oxygen complexes and metalloenzymes, e.g. Ca^{2+} in the Mn_4CaO_5 cluster is indispensable for the catalytic water oxidation in PS II, (although the actual role of calcium remains elusive) and Zn^{2+} in Cu-Zn superoxide dismutases (Cu,Zn-SOD) binding of which to $-superoxide (O_2^{\cdot-})$ facilitates the electron-transfer reduction of $O_2^{\cdot-}$.^[2] Thus, in the biomimetic studies, a Cr(III)-superoxo species bearing a macrocyclic TMC ligand $[(TMC)Cr^{III}(O_2)]^{2+}$ (**1**, TMC = 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane)^[3] has been employed as a prototype of metal-superoxo intermediates for in-depth investigation of its redox-reactivities in the presence of proton (H^+) and other redox-inactive metal ions including Ca^{2+} . A remarkable acid catalysis was observed in oxygen atom transfer (OAT) reactions by **1**, in the presence of triflic acid (HOTf). In the acid-catalyzed reactions, the reactivity of **1** in the sulfoxidation of thioanisole (i.e., OAT reaction) was enhanced greatly, showing more than 10^4 -fold acceleration in the reaction rate. Mechanistic investigation performing kinetic and thermodynamic studies of **1** in electron transfer (ET) reactions using a suitable electron donor in the presence of HOTf (proton coupled electron-transfer, PCET) and different Lewis acidic metal ions (M^{n+} : Ca^{2+} , Mg^{2+} , Y^{3+} , Al^{3+} , and Sc^{3+} ; Lewis acidity (ΔE) of the redox-inactive metal ions is in the order of $Ca^{2+} < Mg^{2+} < Y^{3+} < Al^{3+} < Sc^{3+}$, metal-ion coupled electron-transfer, MCET), revealed that reduction-potential of **1** is hugely dependent on the Lewis acidity of the metal ion used and hence the redox reactivities of **1**. From the Marcus plot analysis it was also found that the reorganization energy of outer sphere-electron transfer from electron donor to **1** varies from 2.32 eV to 2.66 eV depending on the Lewis acidity of the redox inactive metal ions.^[4] Thus, the research work provides valuable insights into the effect of Lewis acidity on the chemical properties and hence the reactivities of the metal-oxygen species relevant to the biological system.

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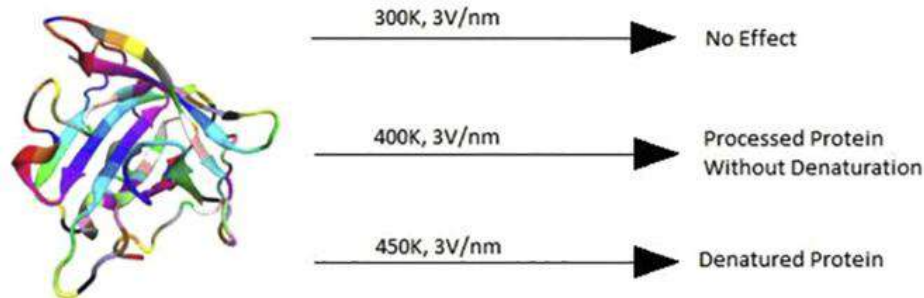
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Structural and functional changes of the protein β -lactoglobulin under thermal and electrical processing conditions

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In the present study we have tried to explore the effect of static external electric field of strength 3.0 V/nm on the conformational changes adopted by the protein β -lactoglobulin. We have chosen different temperatures viz. 300 K, 400 K and 450 K to evaluate the temperature dependent effect of electric field. We have observed that combined effect of high temperature and static external electric field show significant changes on the structural conformation of the protein which in turn may affect the functional properties of the protein. Calculations of root mean square deviations reveal that both helical and β -sheet regions of the protein are noticeably affected at high temperature. We have used solvent accessible surface area (SASA) and dipole moment values to explain that there is changes in hydrophobicity of the protein surface due to presence of external electric field. The study reveals that electric field in combination with high temperature can be used to alter the conformation of the protein and the effect of external electric field is more pronounced at high temperature than that of low temperature. The study provides a better understanding of the conformational changes adopted by the protein under the stress of external electric field and high temperature and provide guidance to choose optimum conditions for processing without loss of nutritional properties.



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Development of strategies for HPLC-free scalable synthesis of unnatural nucleoside triphosphates

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Natural and modified nucleoside triphosphate has brought significant advancement in every major area of healthcare research ranging from DNA sequencing to drug discovery. TNA (Threofuranosyl nucleic acid), one type of XNA (Xeno-nucleic acid) has attracted considerable attention to generate new synthetic polymers having numerous uses in biology, biotechnology and medicine owing to their unique physicochemical properties including increase biological/chemical stability, altered 3D shape and even elevated thermostability for Watson-Crick base pairing. However, the major challenges associated with these nucleoside triphosphates are their scalable synthesis and purification.¹ Although several methods have been developed to get these modified nucleoside triphosphates, these still suffer from scalability and purification issue.² One more challenge associated with the purification is the requirement of HPLC technique that separates the nucleoside triphosphate from other polar side products, but again limited to only a few tens of milligram which is a tedious process in academic labs. So, our target has been to develop new strategies that allows us scalable synthesis of the TNA with convenient silica gel purification. The two mostly followed methods to generate the TNA are the P(V) pyrene pyrophosphate reagent method and iterative process that uses dibenzyl-*N,N*-diisopropylphosphoramidite as the phosphorylating agent. This powerful strategy has led to the synthesis of broad range of natural and unnatural nucleoside triphosphates using protocols that are efficient, inexpensive, and operationally handy.

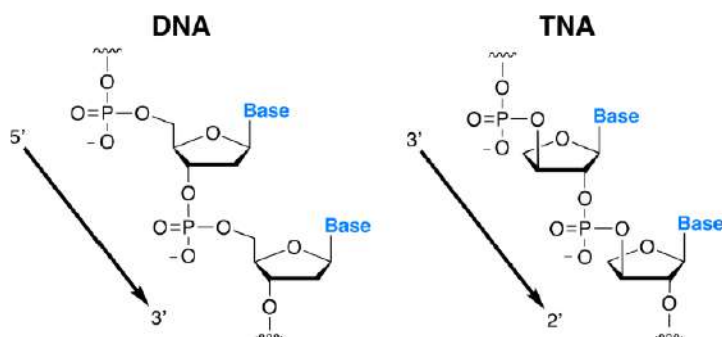


Figure: Chemical structure of DNA and TNA, where DNA maintains strand polarity 5'-3', TNA maintains strand polarity 3'-2' with one less atom per backbone repeat unit than natural DNA

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Development of metal or metal oxide-reduced graphene oxide nanocomposite for their application in the synthesis of industrially important organic compounds

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Graphene oxide, a two-dimensional single layer of sp^2 hybridized carbon atoms arranged in honeycomb lattice, has become one of the most exciting research areas due to its unique nanostructure and properties. Graphene oxide is used as support for the synthesis of metal or metal oxide nanoparticles to prevent the agglomeration of particles which in turn resulted higher surface area. The use of graphene act as not only support material but also it forms a new type of nanocomposite materials with metal or metal oxide nanoparticles. Those nanocomposite materials have enormous applications in diverse fields such as surface-enhanced Raman scattering, catalysis, microelectronics, light emitting diodes, photovoltaic cells and in medical as well as biological applications. Among these, nanocomposite materials for their catalytic application in organic catalysis has attracted particular interest due to high surface area and unique electronic properties of graphene sheets. In addition to these, the π - π interaction between the aromatic moieties of reactant molecules and the graphene support enhances the adsorption capacity of the reactant molecules on to the surface of the catalyst which in turn resulted enhancement in the catalytic performances. Due to such advantageous properties of such nanocomposite materials, they are widely used as efficient catalyst in many catalytic reactions such as reduction of nitroarenes, formic acid oxidation and ethanol electrooxidation, CO oxidation, oxidation of alcohol, degradation of organic pollutants, hydrogenation of C=C and C=O bond, Fisher-Tropsch synthesis and coupling reactions. The coupling reactions are especially important due to their importance of the final coupling product. Coupling reaction like Homocoupling, Suzuki, Sonogashira, A3 coupling and other three component coupling reactions are important organic reactions for the synthesis of industrially valuable compounds like biaryl, biphenylacetylene and other heteroaromatic compounds containing nitrogen atoms such as propargylamine, imidazo[1,2-a]pyridine derivatives etc. Here, in this lecture, the preparation, characterization and application of CuO-reduced graphene oxide based nanocomposite material in the three component coupling reaction for the synthesis of imidazo[1,2-a]pyridine derivatives and propargylamine has been discussed.

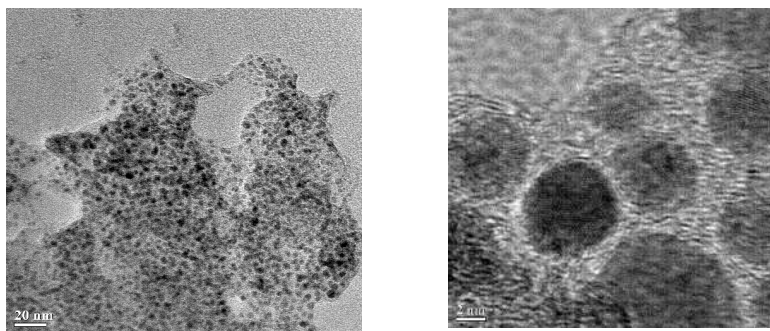


Figure: TEM and HRTEM image of CuO-rGO nanocomposite material

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Medical Devices, Regulatory Pathways to the Market and their Evolution

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History of medical devices goes well beyond centuries when people were realizing how to alleviate a particular disease or other conditions. Over the time our understanding of diseases or other conditions kept improving along with the medical devices as well as the therapeutic techniques. A normal surgical procedure which in this century would take minimum human effort and time used to be a huge surgical miracle in the past centuries. Many therapeutic techniques which are currently being widely practiced were subject of criticism for being nonsensical to the medical community in the past. Few pioneers of modern-day medical science had to sacrifice everything to prove their futuristic innovations which later proved to be lifesaving. However, until late last century, the government health authorities around the world were not realizing that the use of medical devices has to be regulated as although it may alleviate a disease or other condition, but it may also have either long- or short-term minor to fatal effect on the patient. Since their introduction, over the past few decades, medical device regulations around the world are constantly evolving in parallel to the advancement of science and technology as newer information are frequently made available. Additionally, as we have achieved better understanding of human anatomy and responses to certain therapeutic procedures, many previously known information has been revised. With this ever increasing abundance of new information, challenges to the medical device manufacturing communities to introduce modern technologies to the market has also increased as the authorities around the world has tightened their grip on the medical device regulations to ensure their safety and effectiveness.

Determination of surface charge of bio-adsorbent and specific ion effect study

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Keeping in mind about the importance of adsorption and specific ion effect study, surface charge (more specifically, point of zero charge) of three types of bio-based adsorbents namely, “silica (extracted from rice husk ash), cellulose (extracted from banana stem) and a composite made from silica and cellulose” is determined with the help of a simple pH-metric method. Further effect of different inorganic ions (both cations and anions) on the point of zero charge of above surfaces is also explored. The silica and cellulose based adsorbents are characterized by FTIR & XRD techniques. The pH change of the suspensions provide acceptable point of zero charge. Ions with respect to their size and polarizability have been found to affect the surface charge of adsorbents.

Diruthenium Complexes of *p*-Benzoquinone-Imidazole Hybrid Ligands: Innocent or Non-innocent Behavior of the Quinone Moiety

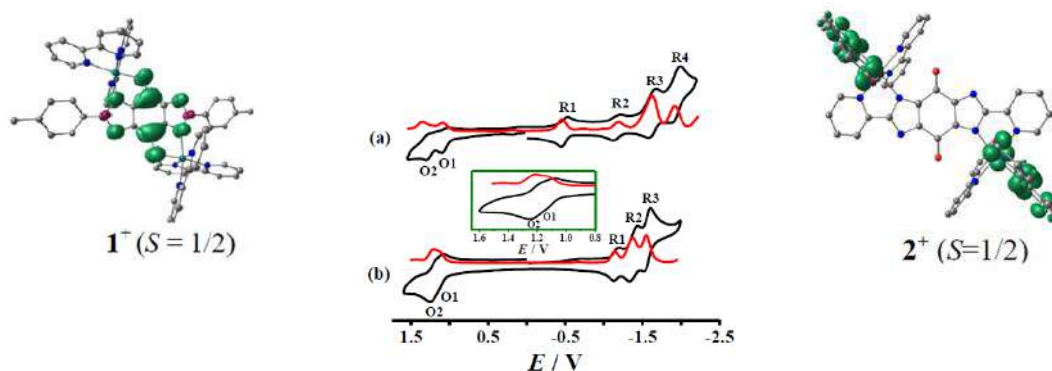
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The inert bonding from ruthenium to heterocyclic N centers has allowed for a great variety of coordination compounds with chelating ligands and various oxidation states of the metal (Ru^{II}, Ru^{III}, Ru^{IV}). In the presence of chelate support ruthenium will also bind to quinone-oxygen atoms, especially when charge can be transferred to this acceptor moiety. Mixed N,O coordinated ruthenium complexes have thus been prepared as mono-, di-, tri-, and tetranuclear species and were studied with respect to structural, electrochemical and spectroscopic properties.¹⁻³ Complexes with two (or more) metal atoms have attracted special interest because of their potential for mixed valency.^{2,3}

In the present contribution, we report two redox non-innocent ligands 2,6-Diaryl-*p*-benzoquinonodiimidazoles (aryl = 4-tolyl, **I**, or 2-pyridyl, **II**) were shown to bridge two [Ru(bpy)₂]²⁺ complex fragments after double deprotonation via imidazolite-N and *p*-quinone-O (**I** → **1**²⁺) or via imidazolite-N and pyridyl-N donor atoms (**II** → **2**²⁺). Characterization by crystal structure analysis, ¹H-NMR spectroscopy, cyclic and differential pulse voltammetry and spectroelectrochemistry (UV-vis-NIR, IR, EPR) in connection with TD-DFT calculations revealed surprisingly different electronic structures for the redox systems **1**ⁿ and **2**ⁿ. Whereas **1**²⁺ is reduced to a radical complex with considerable semiquinone character, the reduction of **2**²⁺ with its exclusive N coordination exhibits little spin on the now redox-innocent quinone moiety in contrast to electron uptake by the pyridyl-imidazolite chelating site. The first of two close-lying oxidation processes is occurring at the bridging heteroquinone ligand while the second oxidation is partly (**1**⁴⁺) or predominantly (**2**⁴⁺) centered at the metals.



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Enhanced electrocatalytic activity of the triply fused binuclear copper porphyrin towards proton reduction: experimental and theoretical insights

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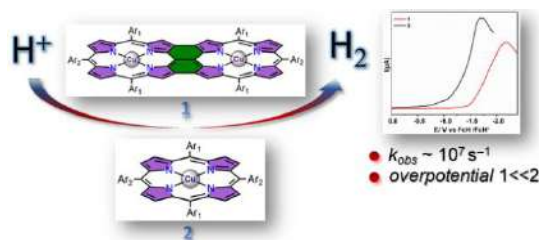
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Limited resources of non-renewable energy, rapid depletion of fossil fuels, and ever-increasing energy demands have emphasized global search for an alternative energy sources.¹

Electrocatalytic hydrogen evolution reaction (HER) ($2\text{H}^{\square} + \text{e}^{\square} \rightarrow \text{H}_2$), a reaction fundamental to various energy transfer related chemical transformation, garnered considerable attention as a new paradigm to the energy storage, delivery and transport.² In this context, transition metal complexes of tetrapyrrolic macrocycles such as porphyrin have come under scrutiny due to unique physical properties and unprecedented reactivity of the metalloporphyrin frameworks. On this ground, several transition metal (Fe, Ni, Co and Cu) complexes of porphyrin have been extensively studied as a HER catalysts.³ While, metal complexes of monoporphyrin have been exploited extensively for electrocatalytic HER, OER and CO_2 reduction reactions, catalytic properties of metal complexes comprising fused porphyrin for proton reduction remains relatively underexplored, barring a sole example of proton reduction by the binuclear doubly fused Cu(II) porphyrins in non-aqueous solvents reported by Moore and co-workers.⁴

In the present contribution, we report an example of HER catalysts based on the triply-fused bimetallic copper porphyrin and draw a comparative analogy of the fused complex's catalytic activity with the analogous monomeric Cu-porphyrin. In comparison to monomeric analogue, triply fused copper porphyrin exhibits higher catalytic activities at lower over potential with a near unity faradic efficiency in DMF in the presence of trifluoroacetic acid as a proton source. Spectroscopic measurements like UV-VIS-NIR/ EPR- SEC have been employed to investigate the electronic structure of the intermediates involved during the catalysis allowing further insight into the mechanistic pathway of the hydrogen evolution process. In addition, theoretical calculations have also been performed to provide further support towards the mechanistic HER behavior of triply fused binuclear copper porphyrin.



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Synthesis, characterisation and catalytic activity of a seven coordinated iron(III)-complex of a phosphorus based N₃P₁ type tris(2-pyridinylamino) phosphinesulphide ligand

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The mononuclear iron complex 1, Fe^{III}(**TPPS**)(Cl)₃, was synthesized using a tripodal tridentate ligand, tris (2-pyridinylamino) phosphinesulphide (**TPPS**), which has three pyridylamino groups attached to a phosphorus atom connected to a sulphur atom (P-S bonded) which can serve as the tridentate or tetradentate ligand for the octahedral Fe(III) ion. The four equatorial positions of the octahedral complex are occupied by two chlorine atoms and two amino N-atoms of two aminopyridyl groups. One of the axial positions is occupied by one chlorine atom and the other position is occupied by the pyridine N-atom of the remaining amino pyridyl group of the ligand. The catalytic activity of the Fe(III) complex has been studied towards the conversion of ketonic functional group to hydroxyl functionality and found to be efficient for more hindered ketonic group. The more acidic behaviour of the N-H proton may be due to the strained four membered ring system in the complex 1.

Key Words: Iron(III) complex, Tripodal ligand, aminopyridyl group, acidic proton, strain ring.

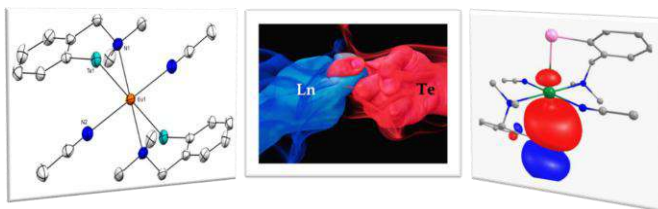
Pushing the Boundary of Covalency in Lanthanoid Ions: Insights from the Synthesis, Molecular and Electronic Structural Studies of Low Coordinate Monomeric Lanthanoid (Eu, Yb) Tellurolates

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Owing to the strict hard/soft dichotomy between lanthanoids and tellurium atoms, and the strong affinity of lanthanoid ions for high coordination number, monomeric lanthanoid tellurolate complexes have remained elusive in comparison to the lanthanoid complexes with lighter group 16 element congeners (O, S and Se).¹ In a first, by utilizing the secondary bonding interaction stabilized hybrid organotellurolate ligands, a series of low coordinate, monomeric lanthanoid (Yb, Eu) tellurolate complexes are reported. In particular, the reaction of bis[2-((dimethylamino)methyl)phenyl]ditelluride² with Ln(0) metal (Ln = Eu, Yb) resulted in the formation of low coordinate, monomeric complexes [Ln^{II}(TeR)₂(Solv)₂] [R = C₆H₄(CH₂NMe₂)-2] [Ln = Eu, Solv = tetrahydrofuran; Ln = Eu, Solv = acetonitrile; Ln = Yb, Solv = tetrahydrofuran; Ln = Yb, Solv = pyridine]. To see the generality of this approach, the synthetic method was extended to 8,8'-diquinolyditelluride³ and the reaction afforded monomeric complexes [Eu^{II}(TeNC₉H₆)₂(Solv)_n] (Solv = tetrahydrofuran, n = 3; Solv = 1,2-dimethoxyethane, n = 2). The europium(II) tellurolate complexes synthesised here represent the first sets of examples of monomeric europium tellurolate complexes. The molecular structures of the complexes reveal that the N→Ln interactions, along with the steric bulk of the ligands, prevent the formation of higher-order aggregates and facilitate the isolation of the desired monomeric species. The electronic structures of the complexes were examined by Density Functional Theory (DFT) calculations, which establish a comparable level of covalency between the lanthanoid and tellurium ions. While the magnetism of europium chalcogenides have gained tremendous attention in contemporary chemistry, the availability of monomeric europium tellurolate species can offer promising opportunities in molecular magnetism.



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Nanoconfined Fluorescent Molecular Container for Live-Cell Imaging and Photodynamic Activity

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In Nature, biological evolution over the time has created a series of natural host with definite spaces, unique geometries, and functionality. Protein-type macrocycle, tubular and cage structures are specially some of those. Biological function of these supramolecular structures is detectable based on its fluorescent property. Synthetically, chemists were able to replicate and mimic these structures to prepare in laboratory which leads to discovery of cyclophane, carbon nanotube and other supramolecular nanoconfined structures. Ever since the first, Bluebox is designed, cyclophane chemistry has been a great interest to chemistry, material, and biological community due to its suitable cavity and optical properties.^{1,2} To mimic natural receptors, we have designed cage like synthetic cyclophane receptor that is tunable to study both in hydrophilic and hydrophobic environment. A series of viability experiments with this synthetic receptor has been studied on breast cancer cells and simultaneously photodynamic therapy has been regulated to kill these cancer cells with a photosensitizer guest with drug activity. In addition to that our study also explores the host-guest recognition with water soluble dye with high binding affinity.

A brief functionality of Stoddart cyclophane chemistry and its application in various field such as material, environmental and biological field will be presented.

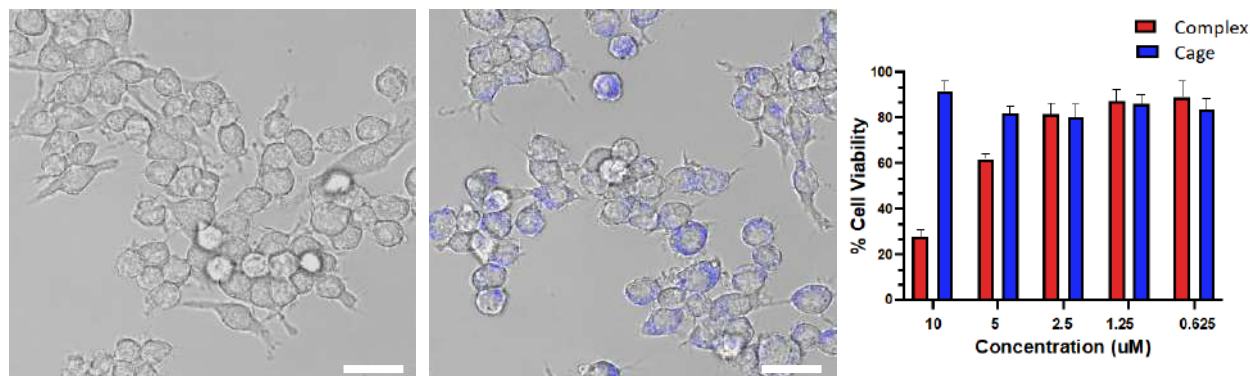


Figure 1: (left to right) Bright field images of breast cancer cells after incubation with precursor and the actual cage and, cell viability after light treatment with the cage and host guest (5,15-Diphenylporphyrin) complex.

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Potato Chemistry: What People Know and What Don't

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Potato is the 4th major food after rice, wheat, and maize in worldwide and America's number one vegetable crop. Potatoes have been portrayed as unhealthy by some nutritionist due to their high starch content. As a result, new varieties of potatoes packed with nutritional and bioactive compounds are being developed. Major nutritional compounds available are vitamins B1, B3, B6, folate, resistant starch, minerals, glycoalkaloids, polyphenols, phenolic acids, and carotenoids. Color fleshed potatoes (purple and red) are rich sources of polyphenols and possess higher level of antioxidant capacity compared to white and yellow fleshed potato tubers. Potato polyphenol compounds has potential role in reducing diabetic complications. Acrylamide, a "probable carcinogen" in French fries and potato chips is a big challenge in potato industry but could be mitigated adopting effective biological and processing technology. In this presentation we are presenting role of potato polyphenolic compounds towards antioxidant capacity, health beneficial properties, and acrylamide formation.

Silver Nanoparticles embedded on *in-vitro* biomineralized Vaterite: A highly efficient catalyst with enhanced catalytic activity towards 4-Nitrophenol reduction

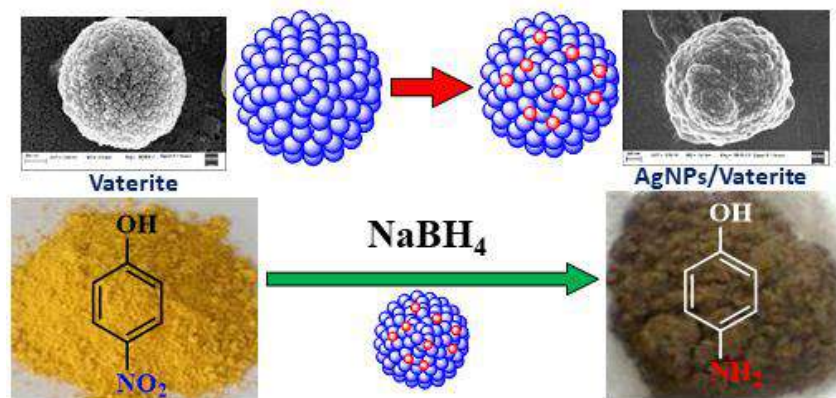
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Biomaterialized vaterite with spherical morphology and a porous surface texture was subjected as the inert solid support for silver nanoparticles to form a composite material that was eventually utilized as a catalyst for the reduction of 4-Nitrophenol. The methods assigned were eco-friendly and one of the highlights was the very even and dense distribution of the silver nanoparticles with no evident signs of agglomeration. The majority of the silver nanoparticles embedded were of ultrafine size, with an average diameter of 3.5 nm. This can be attributed to the porous surface texture of vaterite. The composite catalyst showed excellent catalytic activity and remained unaltered for at least five consecutive cycles. An extension of the study, whereby the effectiveness of the catalyst towards the reduction of 4-Nitrophenol was performed in water from natural sources, showed promising results. Hence, this efficiently designed composite material can be used as a potential catalyst for polluted and wastewater treatment.



Keywords: Biomaterialized Vaterite; silver nanoparticles; composite material; heterogeneous catalysis.

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Stablization of azapeptide and N-methyl azapeptide models from unusual $N_{amide} \cdots H-N_{amide}$ hydrogen bond

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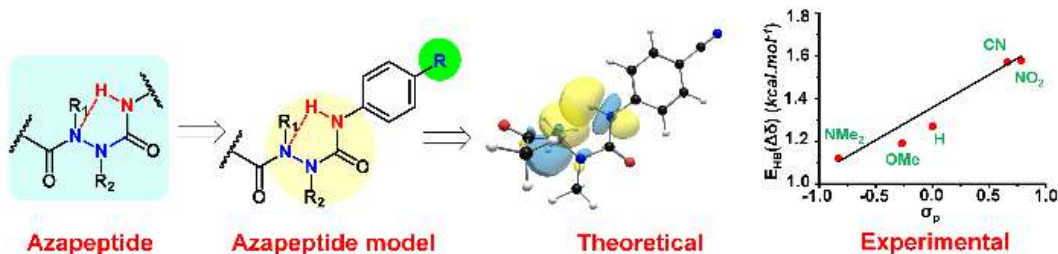
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Azapeptide, wherein the α -carbon atom of a peptide is isosterically replaced with a nitrogen atom in one or more amino acid residues, is an attractive alternative to natural peptide as teurepatic agent due to their improved cell-permeability and enhanced proteolytic stability.¹ In fact, Zoladex and Atazanavir are approved azapeptide-based drugs available in the market.² An unusual $N_{amide} \cdots H-N_{amide}$ hydrogen bond (HB) was previously proposed to stabilize the azapeptide β -turns. Herein, we provide experimental evidence for $N_{amide} \cdots H-N_{amide}$ HB and show that this HB endows a stabilization of 1-3 kcal.mol⁻¹ and enforces the trans-cis-trans (t-c-t) and cis-cis-trans (c-c-t) amide bond conformations in azapeptides and N-methyl-azapeptides, respectively. Our results indicate that these $N_{amide} \cdots H-N_{amide}$ HBs can have stabilizing contributions even in short azapeptides that cannot fold to form β -turns.⁴



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Transport phenomena of self propelled particles, a theoretical approach

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Self-propelled Janus particles are a class of micro-nano sized particles which can move by extracting energy from their surrounding suspension medium. They possess two distinct faces with different chemical or physical properties [1, 2]. Due to self-propulsion, Janus particles can diffuse almost an order of magnitude faster than normal Brownian particles [3].



A Janus particle can tow a passive cargo by binding it to form a self-propelling dimer. Hydrodynamics interaction determine the stable position of the cargo relative to the axis of the active dimer's head. Based on the Langevin description, [4] we proposed a general model which can describe dynamics of any type of self-propelled Janus particles. We show both analytically and as well as numerically [4] that diffusivity of Janus particles strongly depends on the model parameters. Janus particle coupled to a cargo exhibits optimal towing capability only in the puller and pusher configurations, whereas in all other configurations it drives a chiral dynamics, which suppresses the motility of the swimmer-cargo system. Recently we observe the probability of motility transfer from strong self-propeller to weak ones to improve kinetic energy and velocity distribution. We have analyzed the effects of active nano/micromotors with tunable high motility in a suspension of particles whose motility cannot be directly controlled. We showed that by injecting a small fraction of more active Janus particles one can substantially enhance the motility of other less active species. Such a motility enhancement was demonstrated for two typical cases: particles with weak inertia, by studying the velocity distributions for both species, and for overdamped particles, by comparing their effusion rates [6]. Our results would be useful to synthesize Janus particles with desired transport properties for application in nano-technology and medical sciences.

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Unsupported Donor–Acceptor Complexes of Noble Gases with Group 13 Elements

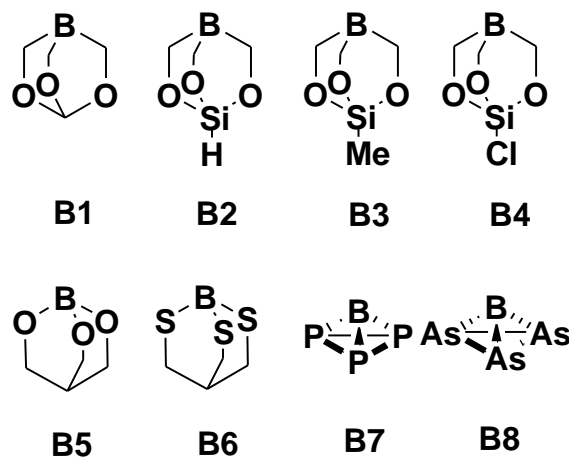
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Unsupported donor–acceptor complexes of noble gases (Ng) with group 13 elements have been theoretically studied using density functional theory. Calculations reveal that heavier noble gases form thermodynamically stable compounds. The present study reveals that no rigid framework is necessary to stabilize the donor–acceptor complexes. Rather, prepyramidalization at the Lewis acid center may be an interesting alternative to stabilize these complexes. Detailed bonding analyses reveal the formation of two-center–two-electron dative bonding, where Ng atoms act as a donor.

Keywords: Pyramidal boron; Donor-acceptor complexes; Theoretical; DFT.



Scheme 1: Pyramidal Lewis acidic boron centres considered in this study

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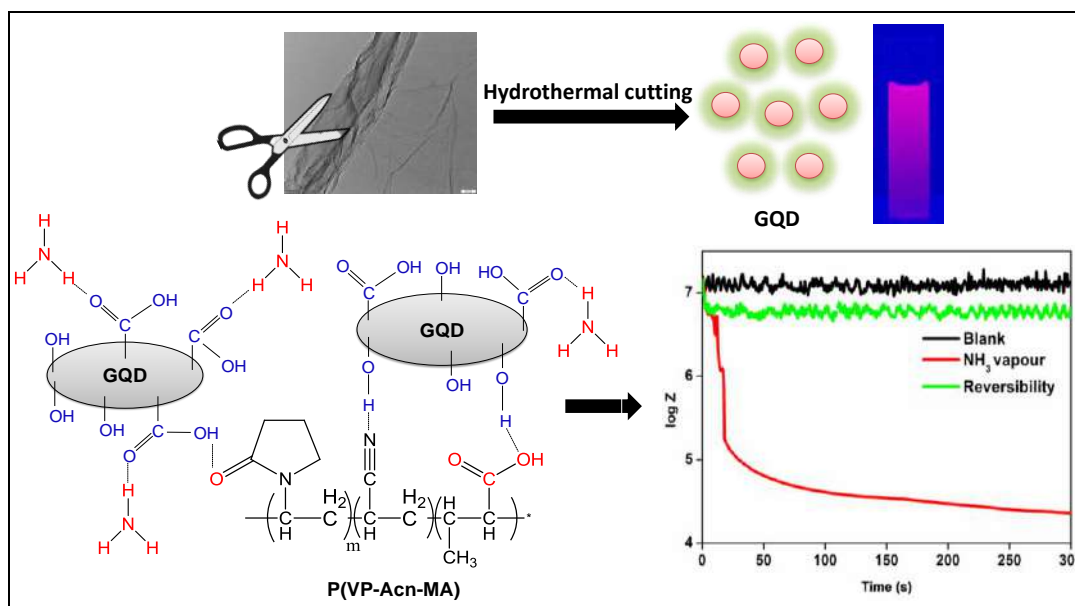
Synthesis and application of Polymer composites as efficient sensing material for the detection of ammonia vapour

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The release of toxic vapours in the environment can cause various respiratory diseases. There are many sources of toxic vapours, such as chemical industries, laboratories, and life-stock, in addition to its natural origin. Hence, the detection of these vapours is of utmost importance. In this work, we present in-situ graphene quantum dot incorporated poly(n-vinylpyrrolidone-co-acrylonitrile-co-methacrylic acid). The polymer composite was found to have enhanced electrical properties compared to the original copolymer. A portable electronic device was fabricated using the polymer composite for the selective and reversible detection of ammonia vapour in the presence of other organic vapours, with a detection limit of 0.225 ppm. The interaction of ammonia vapours with the polymer composite could be attributed to the weak physisorption of the vapour into the polymer matrix. Furthermore, to check the sensor's practical applications, we studied its impedance response in the presence of the gases released from the rotten fish sample. Interestingly, the sensor showed a significant decrease in the impedance which indicates that the polymer composite could be used for the real-time detection of ammonia.



Synthesis of 4-Vinyl-1,2,3,4-tetrahydroisoquinoline from *N*-Tethered Benzyl-Alkenol Catalyzed by Indium (III) Chloride: Formal Synthesis of (±)-Isocyclocelabenzine

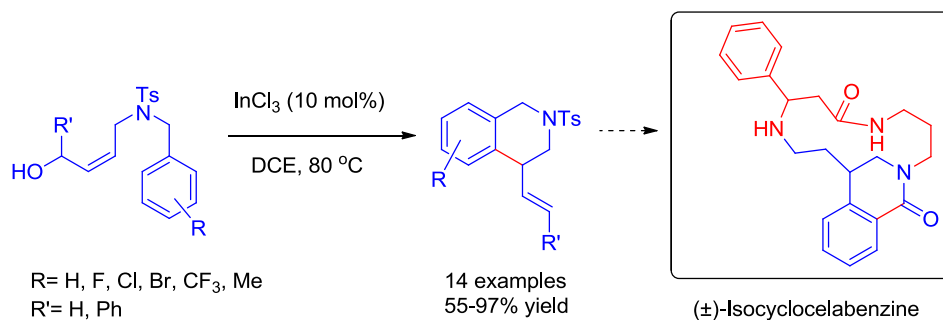
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An intramolecular Friedel–Crafts cyclization reaction catalyzed by indium(III) chloride for the formation of 4-vinyl-1,2,3,4-tetrahydroisoquinoline from *N*-tethered benzyl-alkenol in good yields has been described. The reaction is highly regioselective and generates an exocyclic vinyl functionality in the piperidine ring. The reaction is compatible with a wide range of functional groups. The vinyl functionality is further utilized for the synthesis of 2-(1,2,3,4-tetrahydroisoquinolin-4-yl)ethanol, a precursor for the synthesis of an alkaloid, (±)-Isocyclocelabenzine.



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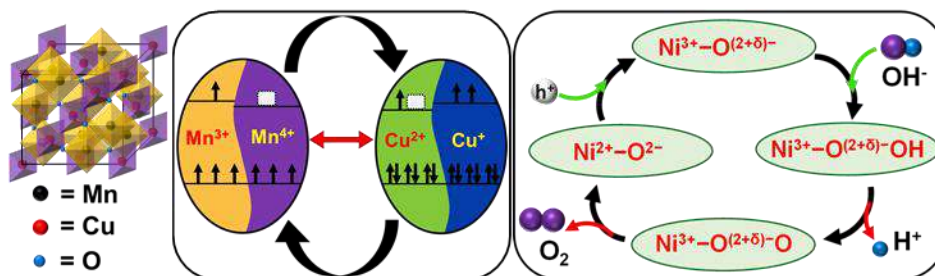
Bimetallic cyclic redox couple in di-manganese copper oxide supported by nickel borate for boosted alkaline electrocatalytic oxygen evolution reaction

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Flake-structured di-manganese copper oxide (Mn_2CuO_4), an unexplored binary-transition metal oxide having mixed-valence states of Mn(III/IV) and Cu(II/I) is utilized as an electrocatalyst for oxygen evolution reaction (OER) and dye degradations. An overpotential of 230 mV @ 10 mA/cm² and Tafel slope of 56mV/decade is achieved with Nickel borate (Ni-B_i) support, which is comparable to the benchmark RuO_2 under similar experimental conditions. Average Faradaic yield of ~98% is achieved indicative of any contribution from the impurities is absent due to the use of alkaline medium. A turnover frequency increased by eight folds is attained with the support of Ni-B_i by virtue of $\text{Ni(II)} \leftrightarrow \text{Ni(III)}$ redox couple. The mechanistic surface kinetics pathway at cross-over potentials between the systems; Mn_2CuO_4 and RuO_2 is studied using electrochemical impedance. The efficiency of the modified catalyst can be attributed to the dual redox cycle of both the di-manganese copper oxide and nickel borate responsible for the charge transfer within the system. Further experiments were performed to check the effect of trace iron impurity in the standard reagent grade chemicals.



Keywords: Oxygen evolution reaction, Electrocatalyst, Redox-couple, Overpotential, Charge transfer process

Reference:

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Synthesis of quinoline based enaminones and studies on their anti-parasitic activities with special reference to antimalarial and anti-filarial activities

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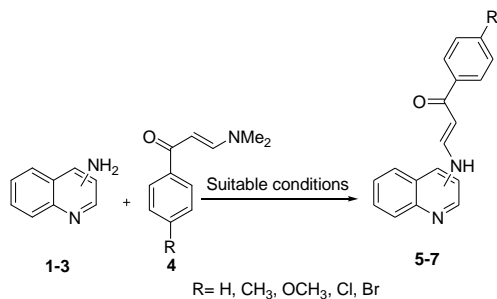
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Quinoline and its derivatives are well known to possess potent anti-parasitic properties, such as anti-malarial^[1], anti-filarial^[2], anti-leishmanial^[3] and some of them i.e.; chloroquine, melfoquine and primaquine^[4] etc are well known drugs for malaria. In connection with an ongoing research programme on the synthesis and biological properties of molecular hybrids consisting of biologically potent molecular entities,^[5-8] we synthesized enaminones of the type **5**, **6** and **7** derived from aminoquinolines [1-3]. Our literature survey at this stage revealed that the anti-parasitic activities of these enaminones are unreported in the literature and hence their biological properties were decided to explore. All the compounds were synthesized in good to excellent yields and the structures have been established with the help of spectral, analytical data and also with the help of X-ray crystallography.



Scheme 1

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Halide Engineering for Mitigating Ion-migration and Defect-States in Hot-casted Perovskite Solar Cells

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Precise control of perovskite morphology to achieve large sized grains with small width grain boundaries is challenging and a pre-requisite for realizing high photovoltaic performance. Ion-migration is another problem with perovskites, which hinders the device results. Herein, incorporation of MABr in mixed halide perovskite $\text{MAPbCl}_x\text{I}_{3-x}$ has been carried out to minimize ion-migration by replacing the mobile I ions in the perovskite with Br^- . Moreover, introduction of MABr results in high quality and smooth films with large grains of average size $\sim 45 \mu\text{m}$. Increasing ratio of MABr was added in the perovskite precursor solution and devices with architecture of FTO/PEDOT:PSS/Perovskite/PCBM/Rhodamine-101/Ag was fabricated using the hot-casting technique. The device with MABr ratio of 0.1 (0.1MABr) showed superior power conversion efficiency of $>18\%$ compared to $\sim 14\%$ of control without any MABr. For higher ratio, performance deteriorated due to the increase in bandgap of the perovskite which resulted in reduction of short-circuit current density. For 0.1MABr minimum defect states and trap density was obtained using various experimental techniques supporting its optimum device performance. Further, minimum recombination loss was taking place in 0.1MABr device. Similarly, the applicability of this technique in large area devices were studied and efficiency of $\sim 17\%$ was obtained which is the highest in literature for devices with 2.5 cm^2 dimensions. This innovative concept and approaches are vital tools to achieve large area grains for increasing the solar cell performance for commercial applications.

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Development of supercapacitors from amine functionalized carbon nanotubes and graphene oxide composite with enhanced specific capacitance

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In this work, the synthesis and supercapacitor electrode fabrication of amine functionalized carbon nanotubes/ graphene composite (rGO/FCNT) has been reported without destroying the 2D structure of reduced graphene oxide sheets. Characterization of the synthesized composite was carried out by SEM, BET and Raman Spectroscopy. The electrochemical analysis of the composite has been performed using cyclic voltammetry, chronopotentiometry and AC impedance spectroscopy technique in a CHI608E electrochemical workstation that revealed a discernible specific capacitance with a noticeable reversibility. Amine functionalities were introduced to the sidewalls of the carbon nanotubes using ethylenediamine as the source of amine group. The final composite was synthesized by in-situ reduction of graphene oxide (GO) in presence of functionalized carbon nanotubes by the addition of hydrazine hydrate. The supercapacitor electrode was then fabricated by dispersing the composite in propanol followed by the addition of nafion. The suspension was then spin coated over stainless steel plate of 1cm². The capacitor evinced a remarkable specific capacitance of 260 F/g at a current density 1 Ag⁻¹.

Key words: *Graphene Oxide, Composite, Specific Capacitance and Supercapacitor.*

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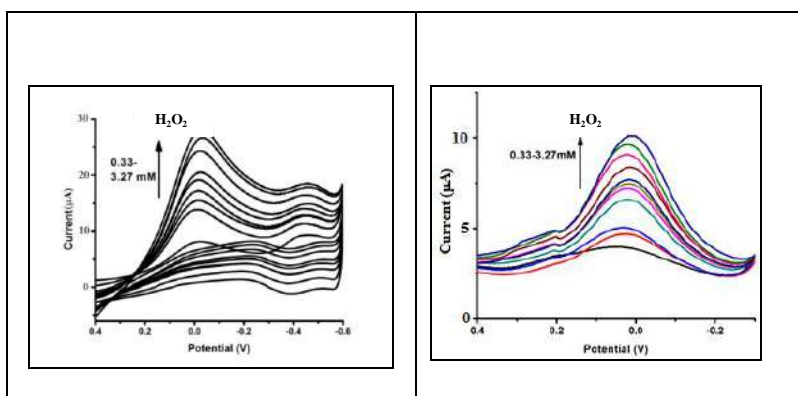
Electrochemical detection of Hydrogen Peroxide using nanoparticle modified Pt-electrode and its biological application

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Hydrogen peroxide is one of the common and simple Reactive oxygen species (ROS) available in nature¹. It acts as signaling molecule in different biological processes and has cytotoxic effects as well². Inappropriate amount of H₂O₂ if present in cells leads to various diseases, even causing death in some cases. H₂O₂ has important role in various aspects such as fuel cell, biotechnology, pharmaceutical, clinical, environmental, industrial research, mining, textile, and food manufacturing (3). Hence the accurate detection and determination of H₂O₂ in cells as well as in environment is of significance. In the present work, AgNPs prepared by a green method using the extract of neem (*Azadirachta Indica*) leaves were used to modify Pt working electrode by repetitive cyclic voltametric scan. The modified AgNPs/Pt electrode could detect H₂O₂ by cyclic voltammetry, square wave voltammetry and electrical impedance spectroscopy (EIS). In cyclic voltammetry, interaction with H₂O₂ shifted the redox potential of the modified electrode in negative direction with gradual increase in the cathodic current while in square wave voltammetry, the peak current increased from 3.909 μ A to 10.09 μ A along with a shift in the potential of AgNP/Pt electrode. The R_{CT} in EIS of the modified electrode was found to increase with the increase in H₂O₂ concentration. No interference was observed for the species- Na⁺, K⁺, Ca²⁺, Mg²⁺, dopamine and ascorbic acid in aqueous medium. AgNP/Pt electrode was also found to detect H₂O₂ in living cells and in BSA-water medium using voltammetric and EIS measurements.



Cyclic voltammogram (left) and Square wave voltammogram plots (right) of the modified Pt electrode at different added concentration of H₂O₂

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Using machine learning to approximate density functionals

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With a rich history of applications, density functional theory (DFT) is often considered a vital component of materials and chemical sciences. From high-temperature superconductors and energy materials to drug design- DFT is the hidden workhorse behind many successful endeavors in these fields. Although DFT is computationally much less expensive than ab initio electronic structure methods, its accuracy depends on the choice of the exchange-correlation (XC) functional, which only exists in approximate form. There are numerous human-designed approximations for this functional that can yield sensible results but with finite accuracy. Routine DFT calculations are also limited to a few hundred atoms due to the computational bottleneck associated with the diagonalization of the Kohn-Sham (KS) equations. Machine learning (ML) has recently made breakthroughs in various applications and is now applied extensively to electronic structure calculations. This presentation will provide a brief account of how supervised ML can lead to a better density functional by improving either the accuracy or the computational cost of DFT. We will especially highlight the construction of a chemically accurate density functional approximation for strongly correlated systems in one dimension with a convolutional neural network to mimic the form of an XC functional within the KS scheme. While the scope of these ML functionals is currently limited, a successful generalization of these approaches to real systems can provide considerable advantages in terms of accuracy and cost and benefit sustainable efforts in all fields.

Surface engineering of Cu-based nanocrystals for electrochemical energy conversion reactions

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The conventional Haber-Bosch ammonia formation method uses H₂ and N₂ at high temperature and pressure. The dependence on natural gas for H₂ production eventually leaves a huge C-footprint. Electrochemical N₂ reduction to ammonia, being a carbon-free process has been an attractive alternative since the past few years. However, lack of selectivity and stability of the catalysts used prevents its industry scale application. We have developed a facile nano architectural engineering on Cu-cubes, forming CuAu hollow beveled nanoboxes to study the electro-reduction of N₂. Interestingly, the CuAu nanoboxes exhibited enhanced NH₃ production than the monometallic counterparts. DFT calculation provides in-depth understanding of the involvement of the Cu-rich inner walls of the CuAu nanoboxes reducing the free energy of the rate-determining step and hence enhancing the catalyst performance.

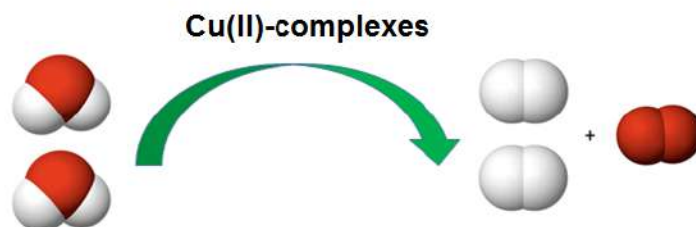
Role of ligand in controlling the electrocatalytic water oxidation activity of Copper complexes

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Development of water oxidation catalysts (WOCs) is an important step towards meeting our future energy demands. Although several WOCs based on readily available transition metals have been reported, Cu-based WOCs have attracted much due to the low cost and biological relevance of Cu.¹⁻³ The first Cu-based WOC was developed by Mayer and co-workers using a mononuclear Cu–bpy system (bpy=2,2'-bipyridine), which induces electrochemical water oxidation under basic conditions (pH 12.5) at an overpotential of approximately 750 mV and with a turnover frequency of 100 s⁻¹. Since then many copper (II)-based WOCs have been reported as competent candidates.^{1,4-6} In this regard we have investigated the electrochemistry of copper complexes with different ligand framework to explore their role in water oxidation activity of the metal complexes.



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Voltammetric electronic tongue with optimized sensors for simultaneous determination of three active pharmaceutical ingredients

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This work uses principal component analysis (PCA) and canonical variate analysis (CVA) in a combination of some clustering metric (F factor) for selection of four optimal electronic tongue (ET) sensors array from a set of eight sensors. PCA and CVA allows to visually compare the performance of the different sensors, while the F factor allows to numerically assess the impact that the inclusion/removal of the different sensors does have in the discrimination ability of the ET towards the compounds of interest. The proposed methodology is based on the measurement of a pure stock solution of each of the compounds under study, and the posterior analysis by PCA/CVA with stepwise iterative removal of the sensors that demote the clustering when retained as part of the array. To verify the potential of such a methodology, the quantification of paracetamol, ascorbic acid and uric acid mixtures were chosen as the study case. Initial sensors array used for the selection of four optimal sensors were seven different graphite epoxy resin (GEC) electrodes modified each of them with cobalt (II) phthalocyanine (CoPc), polypyrrole (PPy), Prussian blue (PB), oxide nanoparticles of bismuth (Bi_2O_3), titanium (TiO_2), zinc (ZnO) and tin (SnO_2) in addition to a Pt disc electrode. An optimal array of four sensors was then derived to build the quantitative artificial neural network (ANN) model. Finally, the performance of the optimized ET was benchmarked against the results previously reported for the analysis of the same mixtures, showing improved performance.

Investment in Science and Technology for Sustainable Development: India's Context

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Investment in science, technology and innovation (STI) is essential for economic development and social progress. Research and development (R&D) can foster sustainable development by building greener, more inclusive societies. To be effective, however, infrastructure development, technology transfer and both public and private R&D need to be nurtured and regulated via effective policies (UNESCO, 2021). The evidence of world economy shows that the developed countries are spending huge sum of money in science and technology. By investing in research and development, these countries innovate cut throat technology, improved their living standards and ruled on poor countries. India, although makes progress in many fields of science and technology, yet a technologically backward country in general. India's expenditure on science is very low in comparison to developed countries. As per Economic Survey 2021, India's gross domestic expenditure on R&D (GERD) as a percentage of GDP stood at 0.65%. The result is that India ranks 48th in global innovating index and 117th in sustainable development goal (SDG) index. On this background, this paper tries to examine the investment pattern of India on science and technology. It also highlighted the consequences on society because of low investment on science and technology.

Key Words: Science, Technology, Innovation, Investment, Sustainable

Domino Synthesis of Tricyanovinylindoles from *o*-Alkynylanilines utilizing DMSO as One-Carbon Synthon

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An effective one-pot Pd(II)/Cu(II) catalyzed domino synthesis of tricyanovinylindoles has been from *o*-alkynylanilines and malononitrile is achieved in the presence of NH₄SCN and NBS in DMSO at 110 °C. The reaction proceeds via Pd(II) catalyzed intramolecular construction of 2-aryl indole followed by Cu(II) catalyzed methyl radical addition from DMSO and subsequent oxidation to give 2-aryl-3-formyl indole. The tricyanosubstituted vinyl moiety is achieved by sequential addition of malononitrile and CN (from ammonium thiocyanate) to 2-aryl-3-formyl indole resulting into two C-C, one C=C, and one C-N bond. Photophysical studies of selected compounds display emission in the visible range.



Green synthesis of Silver Nanoparticles and its Application on Catalytic Degradation of Methylene Blue

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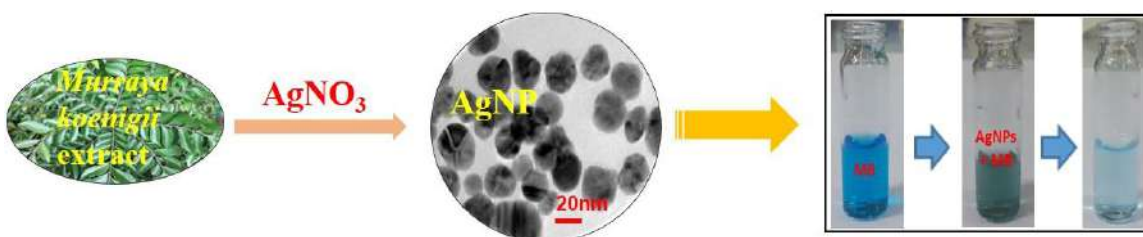
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The present work described an eco-friendly room temperature green synthesis of biocompatible silver nanoparticles (AgNPs) by the reduction of silver ions (Ag^+) using *Murraya koenigii* leaf extract. Synthesized AgNPs were characterized by UV-visible absorption spectroscopy, FTIR, XRD, dynamic light scattering (DLS), Zeta potential (ζ), high resolution transmission electron microscopy (HRTEM) and energy dispersive X-ray (EDX) studies. Synthesized AgNPs could act as photo catalyst for the degradation of methylene blue (MB) dye.

Keywords: Green synthesis, Silver nanoparticles, UV-visible absorption spectroscopy, photocatalysis.

Graphical Abstract:



Efficient Trap Passivation of MAPbI₃ via Multifunctional Anchoring for High-Performance and Stable Perovskite Solar Cells

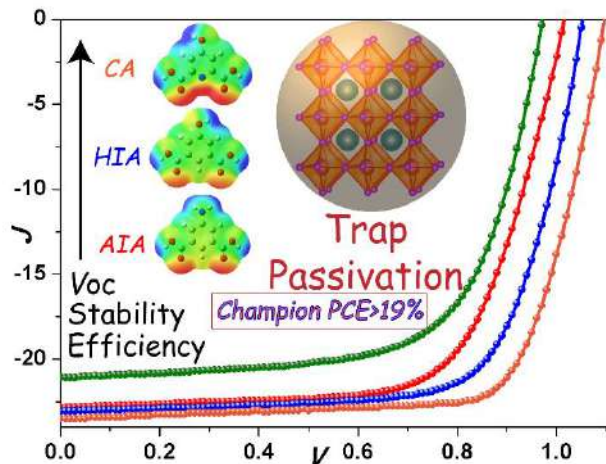
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Chemical passivation of ionic defects in perovskite materials (especially in the surface and grain boundaries) is an effective strategy to reduce charge recombination in perovskite solar cells (PSCs).¹ Despite reports of several additives being used for this purpose, it is very difficult to attribute a specific role for these additives since the passivation mechanisms of different functional groups remains very unclear. Herein, the effect of molecules possessing multiple functional anchoring has been systematically investigated. Three different multifunctional molecules namely 5-aminoisophthalic acid (AIA), 5-hydroxyisophthalic acid (HIA) and chelidamic acid (CA) have been strategically chosen. These molecules not only take part in crystallization process but also passivate the trap states effectively. CA molecule shows superior passivation capacity among all with its better dipolar electron density distribution. The passivated films revealed considerably improved morphology with lesser pin holes and larger grains in comparison to the pristine film. These passivation molecules, having multiple functional groups, have been shown to simultaneously passivate all kinds of defects (cationic and anionic) of perovskite very efficiently. CA passivated p-i-n structured photovoltaic devices have demonstrated the best PCE of 19.06% with an impressive V_{OC} of 1.097 V, an improvement of 125 mV over the device without passivation that showed a PCE of 13.60% and V_{OC} of 0.972 V. Moreover, the devices reveal notable thermal and ambient stability in comparison to the pristine devices due to lower defect states and reduced ion migration.



Synthesis and Photophysical Study of a Pyrene-labeled Dual Emitting Fluorescent Nucleoside

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Understanding the biological events associated with inter-biomolecular interactions, such as dielectric properties in DNA, proteins, cell membranes and structures, functions, dynamics of biomolecules is a very indispensable research area in current years. In this respect, highly solvatochromic fluorescent probes and fluorescently labeled biomolecular building blocks such as solvofluorochromic nucleosides/ amino acids have been successfully utilized for the sensing and detection of such biomolecular events. Toward this end we report the rational design and synthesis of a few fluorescently labeled C5-substituted 2'-deoxyuridines. The synthesized nucleosides have shown interesting solvatochromic characteristic and/or intramolecular charge transfer (ICT) feature. Few of them also exhibit dual emitting characteristics evidencing our designing concept. In an extensive photophysical study, our pyrene-labeled nucleoside, ^{PMAPTPyU} revealed a strong binding interaction with BSA protein.

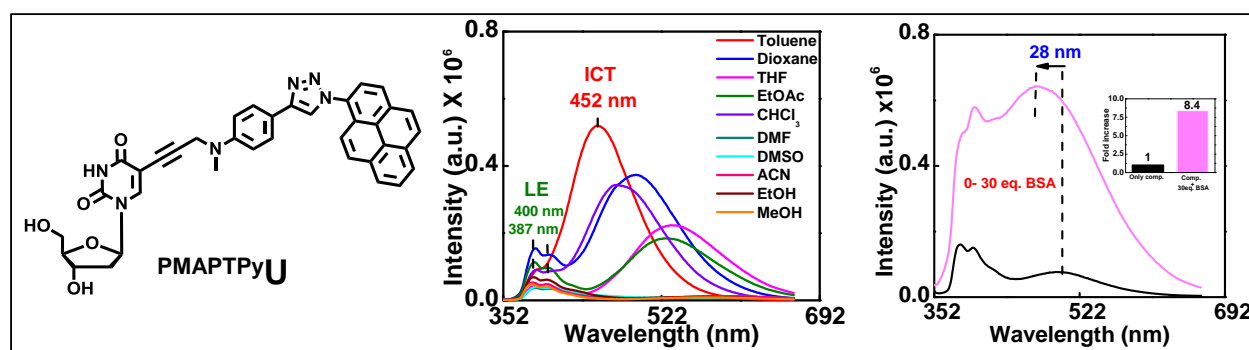


Figure 1. The structure of the synthesized pyrene-labeled nucleoside, its dual emitting property in various organic solvents and its interaction with BSA protein.

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Impact of climate change on the Sustainable development of Assam

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Climate change is a global phenomenon affecting every nation. It is very likely caused by the emission of greenhouse gases from human activities, and poses significant risks for a range of human and natural systems. Now days the climate change or global warming has aroused the attention all over the world, because not only can it directly damage the living environment, but it can also impact on the social and economic development, of a country in an obvious and far-reaching. In this paper, I used the trans-log production function model incorporating variables, such as rainfall, labour force, technology and temperature to stimulate how climate changes impacted on the regional economics. Time series data of the domestic economy of Assam, between 1991 and 2019, were used to verify the production theory of trans-log production frontier. It is found that, with the rainfall increased and temperature declined the climate impact on the economy and absolute value of the output elasticity of the frontier diminished. In addition, the climate change was also positively related to the capital investment. The larger variation of temperature negatively impacted on the economic development.

Key Words: Climate Change, Tras-log production Frontier, global warming, Economic development

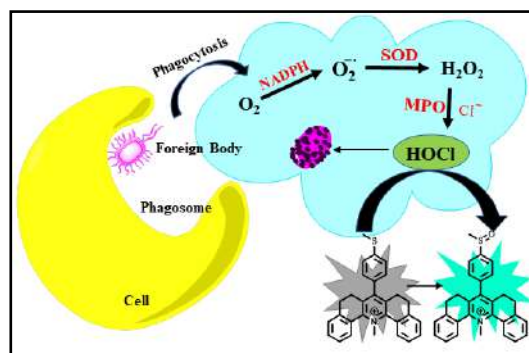
PET based a unique pyridinium fluorescent probe for imaging of hypochlorite (HOCl) in NOX2 pathways for monitoring immune defense

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The human innate immune system is responsible for eliminating pathogens or external species through phagocytosis. This process usually occurs by activating the Nicotinamide adenine dinucleotide (NADPH) oxidase via the NOX2 pathway where the generated peroxide reacts with Myeloperoxidase (MPO) and chloride ions to produce HOCl¹. However, in this process sometimes the concentration of HOCl, a class of reactive oxygen species (ROS) increases which causes oxidative stress



leading to cell death. The adverse effects of HOCl are highly associated with cardiovascular disease, neurodegenerative disorders, acute lung injuries, inflammatory diseases, and cancer². Thus, the monitoring of ROS by a simple, accurate, and reliable method is very much crucial for a normal and healthy immune defense. A fluorescent probe which is used for sensing an analyte producing a detectable change of a signal has been an active area for research in the last two decades. Fluorescent probes have revolutionized the understanding of biological systems through their selectivity, sensitivity, and fast response to specific analytes^{3,4}. Thus, herein, we synthesized a PET based probe, named as **PM-OC** that exhibited fast response (within seconds), high sensitivity (~ 50nM), high selectivity against relevant 30 analytes, and large fluorescence enhancement upon reaction with HOCl. Moreover, we applied our probe to study the biological processes by inducing and inhibiting HOCl production via the NOX2 pathway in both HepG2 and HeLa cells. This mechanistic understanding may offer an advanced platform for monitoring the immune system more accurately especially on NOX2 pathways.

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Vinylsilanes in Highly Diastereo- and Regio-Selective Synthesis of Dihydropyrans

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An efficient strategy for the synthesis of dihydropyrans from silyl-homoallylic alcohols and aldehydes is presented. The dihydropyrans are reported in moderate to good yields. The reaction proceeds via concerted oxonium-ene and stepwise oxonium-ene reactions. The oxonium-ene cyclization process provides single regio-isomeric products, whereas stepwise oxonium-ene reaction gives a mixture of regio-isomers. The reaction is also diastereo-selective. The reaction faces the limitation that it gives the regio-isomeric mixture with aliphatic aldehydes and aromatic-substituted secondary homoallylic alcohols.



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Analysis of Nutrient Content of Some Underutilized Green Leafy Vegetables (GLV) of Assam

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North Eastern region of India is rich in flora and fauna. The people of this region are traditionally using different types of wild plants as food and as folk medicine since ancient time. Ethno-botanical studies have reported that 200 plant species from Arunachal Pradesh, 286 plant species from Assam, 834 plant species from Meghalaya, 526 plant species from Nagaland and 194 plant species from Tripura are used for treatment of different diseases and ailments in these states (1). These plants are available seasonally, and practically a very little information is available on the nutrient content of such vegetables. Leafy vegetables are the least expensive sources of minerals, fibres, vitamins, carbohydrates, proteins and amino acids. GLV are known to be rich sources of micronutrients as well as dietary fibre. Micronutrient malnutrition is one of the major concerns in India and other developing countries. Locally available GLV, which are inexpensive, can be used in the diets to eradicate micronutrient malnutrition. The present study was undertaken with the objective of exploring some wild GLV grown in Assam and to analyse the nutrient composition of the same. The minerals ranges (mg/100g) were: Na (6.7 -15.7), K (132.8 - 212.4), Ca (178.8 - 478.7), Mg (27.6 -178.8), P (31.3 - 47.9), Fe (5.2 - 17.8) and Zn (0.27 - 0.78). Moisture, ash, protein, lipid and carbohydrate of the vegetables were in the range of 86.5 - 92.7, 1.81 - 2.64, 2.13 - 3.34, 0.07 - 0.13 and 4.13 – 7.14 g/100g respectively. Total, insoluble and soluble dietary fibre content of the vegetables ranged from 3.12 to 4.82, 2.62 to 4.21 and 0.41 to 0.65 g/100 g respectively.

Keywords: Green Leafy Vegetables, nutrient Content, dietary

Reference:

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RHIZOSPHERIC FREE-LIVING DIAZOTROPHS IN ACIDIC RICE AGRO-ECOSYSTEM SOILS OF ASSAM, INDIA

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Research and exploration of diverse plant growth-promoting rhizobacteria (PGPDR) has gained priority to ensure sustainable agriculture and future food security to combat issues of climate change. In this regard, efforts have been made to exploit the novel strains of free-living nitrogen fixing rhizobacteria (diazotrophs) from the acidic lowland rice agro-ecosystem soils of Assam for using these strains as biofertilizers for various economically important crops. In the present study, twenty species of free-living rhizospheric diazotroph viz., *Achromobacter xyloxidans*, *Acinetobacter johnsonii*, *Acinetobacter radioresistans*, *Alcaligenes faecalis*, *Azospirillum amazonense*, *Azotobacter chroococcum*, *Beijerinckia indica*, *Burkholderia caribensis*, *Bacillus polymyxa*, *Derrxia gummosa*, *Enterobacter cloacae*, *Gluconacetobacter liquefaciens*, *Herbaspirillum rubrisubalbicans*, *Herbaspirillum sp.*, *Klebsiella pneumonia*, *Pantoea agglomerans*, *Pseudomonas fluorescence*, *Pseudomonas putida*, *Sphingomonas azotifigens*, and *Stenotrophomonas maltophilia* were isolated from rhizospheric soils of lowland acidic rice agro-ecosystems of Assam, India. Among these twenty species, *A. amazonense*, *A. chroococcum* and *B. caribensis* have higher rhizospheric population. The isolated bacterial species were screened for the acetylene reduction, production of indole 3-acetic acid (IAA), phosphate solubilisation, zinc solubilisation, sulphur oxidation, 1-aminocyclopropane-1-carboxylate (ACC) deaminase activity and siderophore production. Acetylene reduction activity and IAA production were higher in case of *A. chroococcum* and *A. amazonense*. Species of *A. chroococcum*, *A. amazonense*, *G. liquefaciens*, *S. azotifigens*, *A. xylosoxidans*, *P. agglomerans*, *P. putida*, *Herbaspirillum sp.*, *K. pneumonia*, *B. polymyxa* and *P. fluorescence* were tested positive for phosphate solubilisation. *P. putida*, *G. liquefaciens*, *Herbaspirillum sp.*, *P. fluorescence* and *B. polymyxa* have been tested positive for zinc solubilisation and sulphur oxidation. *B. caribensis* have shown highest ACC deaminase activity and produced hydroxamate type of siderophore. All the isolated species are gram negative except *B. polymyxa*. Most of the strains are catalase and oxidase positive. All the isolates showed nitrogen fixing activity in Burk's media. *A. chroococcum*, *A. amazonense*, and *B. indica* produced PHB granule and cyst. The findings of this study indicate that most of the isolated diazotroph strains possess multiple PGP properties that have the potential to significantly improve the growth and yield parameters of rice as microbial inoculants or biofertilizers in lowland acidic rice agro-ecosystems of Barak Valley region of Assam, India.

Keywords: Diazotrophs, Siderophore, Rhizosphere, Free-living, Biofertilizers.

Transition Metal Catalysed C-H Functionalization/Oxidative Annulation: Access to Multifunctional Luminogens

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Transition metal catalysed C-H functionalization and annulation have become one of the major focus of research because of its atom and step economical pathway¹⁻²; thereby leading to an assortment of fused polyheterocyclic scaffolds. These polyheterocycles are widespread in nature and possess several interesting biological activities. Besides biological activities, they also exhibit outstanding luminescence and photophysical properties. These luminescent materials display various photophysical phenomenon including Aggregation-induced emission (AIE) and have wide application in “turn-on” or “light-up” biosensors or chemo sensors, DNA visualizers, specific imaging of cancer cells, tissues, bacteria, etc.

The idea of introducing a new functionality, formation of a new C-C bond or a resonance stabilised annulation product via direct C-H bond transformation is a highly attractive strategy in the field of covalent synthesis. The library of substrates is virtually unlimited, including complex organic compounds, drugs molecules, synthetic and biological polymers. Transition metal catalyzes transformation of these substrates to a vastly superior class of compounds in an atom and step economical protocol. In this scenario, the use of earth abundant, less toxic and cheaper 3d transition metal is a cherry on the cake (Figure 1).

In 2019, our group developed a library of multifunctional quinoxalium AEEgens via ruthenium catalyzed oxidative annulation reaction of 2-arylquinoxalines with internal alkynes³ (Figure 2). In this report, we investigated the mechanism and detailed applications of AEEgens including mechanochromism, development of latent fingerprints as well as proliferative activity of such AEEgen towards cancerous cells. The synthesized annulated quaternary ammonium salts emit light in green to yellow region.



Figure 1

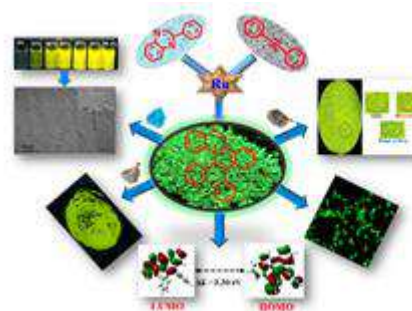


Figure 2: Multifunctional AEEgens

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Degradation of Wetlands in Assam: Challenges and Measures for Sustainable Development

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Wetlands have been identified as one of the most important natural resources of earth. Wetlands are unique and productive ecosystem acting as sources to diverse flora and fauna, synchronizing regional climate, providing natural sinks, maintaining water quality, and transforming a multitude of chemical, biological and generic materials. The state of Assam is bestowed with numerous numbers of wetlands comprising a total area of 764372 hectares that accounts for 9.74 % of the total area of the state as per the National Wetland Atlas (NWA) published by ISRO. In Assam, such wetlands have different names such as *beel, jalah, dalani, pitoni, doba, hola, pukhuri, haor, gadeng* etc. The role of these wetlands in flood management and enriching the biodiversity are many. Wetlands with their plant and animal life provide subsistence for millions of inhabitants in the vicinity. Moreover, these wetlands have been acting as a source of livelihood for many people living in the neighbouring villages. Unfortunately, these wetlands are gradually disappearing due to various reasons particularly in the recent past. The ever-increasing population growth supplemented with industrial and agricultural expansion resulted in the shrinking of area of wetlands and disappearance in many major wetlands of Assam. The present study aims at to assess the current status of the wetlands of Assam, its changing scenarios and various challenges and probable measures in rejuvenating the wetlands in terms of its ecological services as well as to ensure sustainable livelihood for the people dependent on it.

Keywords: Wetland, Assam, biodiversity, disappearing, rejuvenating, sustainable

Synthesis of a Novel MOF Based on Fumarate Bridges and 4,4'-bipyridine Spacers

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A new metal organic co-ordination framework formulated as $\{[\text{Co}_2(\text{fum})_2(4,4'\text{-bpy})(\text{H}_2\text{O})_2].2(4,4'\text{-bpy})\}_n$ has been prepared and structurally characterized. Each pair of Co(II) are bridged by fumarate ligands to form chains which are cross linked by bridging bidentate 4,4'-bipyridine ligand to form a 3-D co-ordination framework. Metal center shows a distorted octahedral environment formed by three oxygen atoms from three asymmetrically coordinated fumarate ligands and two nitrogen atoms from two trans-coordinated 4,4'-bipyridine molecules and one oxygen atom from aqua ligand.

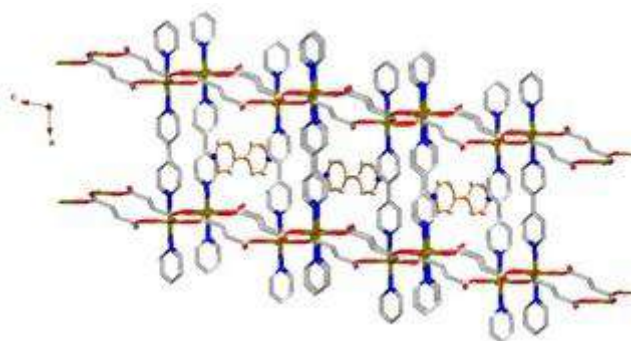


Fig: 3-D framework of the complex viewed along y-axis showing the guest 4,4'-bipyridine molecules in the ball and stick mode (hydrogen atoms are omitted for clarity)

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Oxidation of 2-chlorophenol in water over Co(II)- impregnated SiO₂ catalyst**Ananya Das and Hrishikesh Sarma***Department of Chemistry, B.Borooh College, Guwahati, Assam, India**Email: ananyaluku@gmail.com*

Phenol and substituted phenols are considered as one of the major groups of organic pollutants that are known to have adverse effects to human health and the ecosystem in general. These pollutants are discharged into water mainly from industrial sources and being refractory in nature, they present a major environmental problem. These compounds are resistant to biological oxidation in the conventional effluent treatment plants of the industries and therefore, have been termed as refractory in nature. However, they continue to be released to the aquatic environment from various sources and an urgent need exists for devising suitable methods to remove these materials from water either by complete mineralization or by transforming them to some simple compounds which are biodegradable. Catalytic wet peroxide oxidation (CWPO) method is found to be very promising in this regard.

In the present work, Co(II) was impregnated into silica (SiO₂) and the material was used as a catalyst for oxidation of 2-Chlorophenol(2-CP) in water with the oxidant, H₂O₂. The impregnation was carried out by refluxing acid treated silica with Cobalt(II) nitrate hexahydrate for 6 hr. The catalyst was characterized by FTIR, powder XRD, TGA, SEM and CEC measurement. The amount of metal entering into the silica matrix was estimated using AAS. The material was calcined at 873 K before using as an oxidation catalyst. The oxidation reactions was carried out in a high pressure stirred reactor under various reaction conditions such as effect of P^H, reaction time, temperature, mole ratio of reactants, reactant concentration, catalytic load. The experimental results indicate that the use of this catalyst allows a satisfactory removal of 2-chlorophenol (93.7%) and a significant removal of chemical oxygen demand (60.1%) with a temperature range up to 323K, catalyst load 2g/L and 2-CP: H₂O₂ mole ratio of 1:1. Furthermore, oxidation of the reaction followed second order kinetics. The results shows that Co(II)-impregnated silica produces very effective catalyst for wet peroxide oxidation of 2-Chlorophennol.

Keywords: CWPO, 2-CP, Impregnation, SiO₂, Cobalt (II) nitrate hexahydrate.

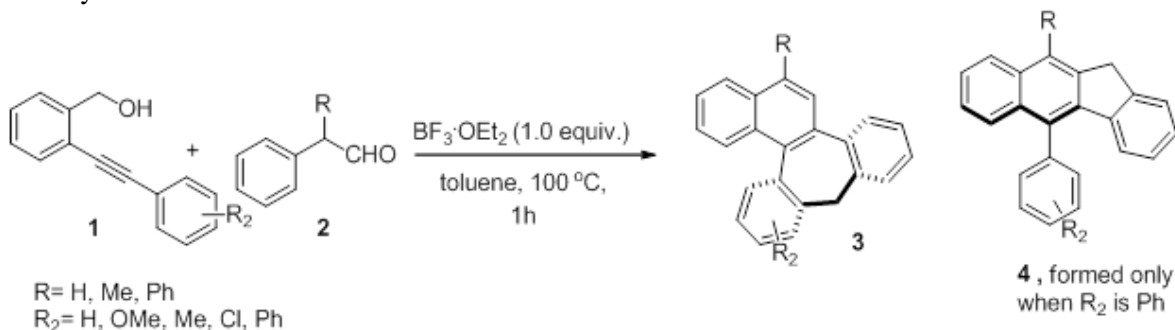
Tandem electrophilic addition and double Friedel-Crafts reactions: An Access to dibenzo cyclohepta[1,2-a]naphthalene derivatives

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Dibenzocycloheptane is an important structural motif also encountered in some biologically active molecules.¹ A simple methodology has been developed for the synthesis of substituted 9H-dibenzo[3,4:6,7]-cyclohepta[1,2-a]naphthalenes from phenylacetaldehydes and ortho-alkynyl benzyl alcohols in presence of Lewis acid in moderate to good yields within a short reaction time.² Interestingly, the reaction proceeds through a highly regioselective electrophilic addition followed by double Friedel-Crafts reaction to form uncommon dibenzo-fused-seven membered carbocycles. The compounds formed are axially chiral and exist as enantiomers in ratio of 1:1 as conformed from HPLC.



Scheme 1

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Visible Light Mediated Thiolation of Substituted 1,4-Napthaquinones Using Eosin Y

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An efficient, one-step procedure for thiolation of substituted 1,4-Napthaquinones (1,4-NQ) was carried out in presence of green LED light (530 nm) using Eosin Y (EY) as photoredox catalyst at room temperature (RT). Thiyl radical generation was the rate determining step and it was characterized by HR-MS technique. Cost effectiveness, operational simplicity, short reaction time, high atom economy and very good yield makes this photoredox-mediated process is a useful alternative to the direct coupling reaction of quinones with thiols or disulphides with transition metal (Cu, Ag and Pd) catalyst.

A Fluorescent "Turn-On" Sensing Of Cerium (III) Based On The Condensation Product Of 4-Methoxybenzaldehyde And Ethylenediamine

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The condensation reaction of 4-methoxybenzaldehyde and ethylenediamine gives **L**. **L** can detect Ce^{3+} by fluorescence "off-on" mode in methanol at $\lambda_{\text{ex}} = 270\text{nm}$. **L** shows a 33-fold enhancement of its fluorescence intensity in methanol upon interacting with Ce^{3+} with $\lambda_{\text{max}} = 360\text{nm}$, when excited with 270nm of photons. The interaction between **L** and Ce^{3+} is free from the interference of metal ions such as K^+ , Na^+ , Co^{2+} , Hg^{2+} , Cd^{2+} , Ni^{2+} , Zn^{2+} , Mn^{2+} , Mg^{2+} , Ca^{2+} , Al^{3+} etc. The stoichiometry of binding and binding constant were calculated from spectroscopic data and it is found to be 1:1 and $10^{4.8}$ respectively. The detection limit was calculated and it was found to be $10^{-5.2}\text{M}$. The binding of Ce^{3+} to **L** was found to be reversible with respect to Na_2EDTA . The mechanism of fluorescence intensity enhancement in the **L** upon interaction with Ce^{3+} can be well explained on the basis of photoinduced electron transfer (PET) mechanism.

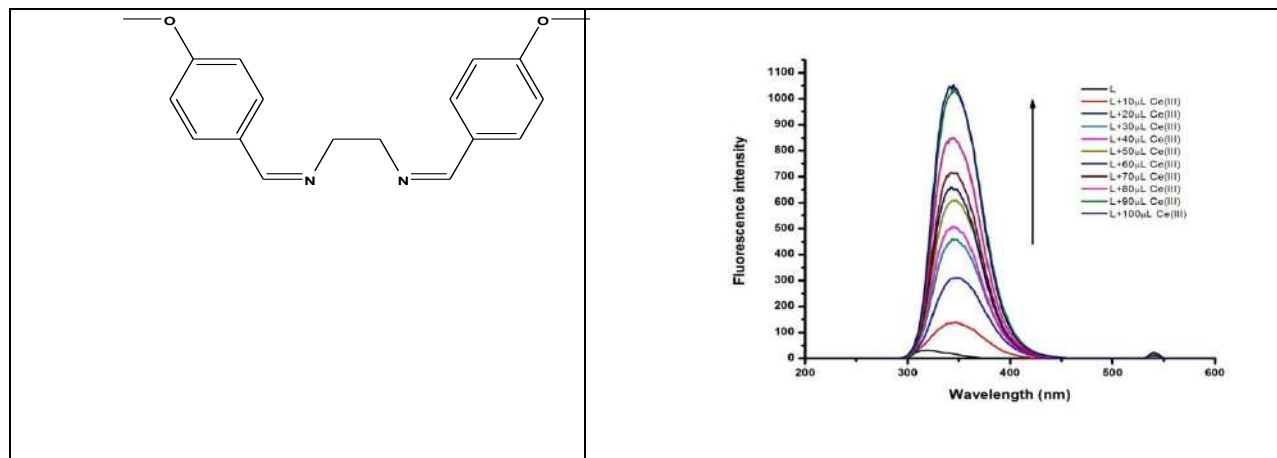


Fig: Structure of **L** (left) and fluorescence spectra of **L** in methanol at different added concentration of Ce^{3+} . $\lambda_{\text{ex}} = 270\text{nm}$, $\lambda_{\text{max}} = 344\text{nm}$.

A Comparative Study on the Structural, Morphological and Photophysical Properties of Chemically Synthesized ZnS and Mn doped ZnS Nanoparticles

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Herein, we study the structural, morphological and photophysical properties of ZnS and Mn doped ZnS nanosized particles synthesized by a simple and effective chemical method. XRD and TEM analysis was used to confirm the formation of nanosized ZnS and Mn doped ZnS particles. The as synthesized ZnS nanoparticles were found to be of spherical shape with size ~ 6 nm (average) whereas Mn doping was found to decrease the size of the nanoparticles further. To get an insight of the morphology, thin films of the nanoparticles were prepared and FESEM and AFM analysis were carried out. FESEM analysis revealed uniform morphology of the nanosized particles along with formation of clusters due to agglomeration. Surface roughness of the films was observed using AFM analysis and it was found to reduce with increasing Mn doping percentage in ZnS. The photophysical properties of the ZnS and Mn doped ZnS nanostructures were studied using UV-vis and PL analysis. The absorption peak in the UV-Vis spectra was blue shifted and increase in band gap of ZnS was observed which can be attributed to the quantum confinement effect. This blue shift was found to increase with increasing Mn doping percentage in ZnS (0.06-0.17 eV). Moreover, while the PL spectra of undoped ZnS showed the characteristics blue peak of ZnS, the presence of yellow/red peak was observed for Mn doped ZnS nanoparticles.

Keywords: ZnS, ZnS:Mn, blue shift, nanoparticles, quantum confinement effect

Stereoselective Synthesis of 4-O-Tosyltetrahydropyrans via Prins Cyclization Reaction of Enol Ethers

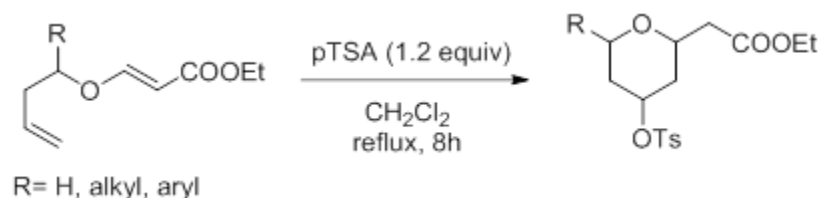
Sujit Sarkar, Namita Devi, Bikoshita Porashar, SantuRuidas and Anil K Saikia*

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A strategy for the stereoselective synthesis of tosyl substituted tetrahydropyrans through Prins cyclization reaction of acryloyl enol ethers has been developed. In this methodology, paratoluene sulfonic acid act as a nucleophile and activator in Prins cyclization reaction of acryloyl ethers. The reaction is highly diastereoselective giving good yields. This methodology will also be useful for the synthesis of other substituted pyran rings such as 4-iodotetrahydropyrans and 2,6-disubstituted tetrahydropyrans by substitution or reduction of the tosyl functionality, respectively.



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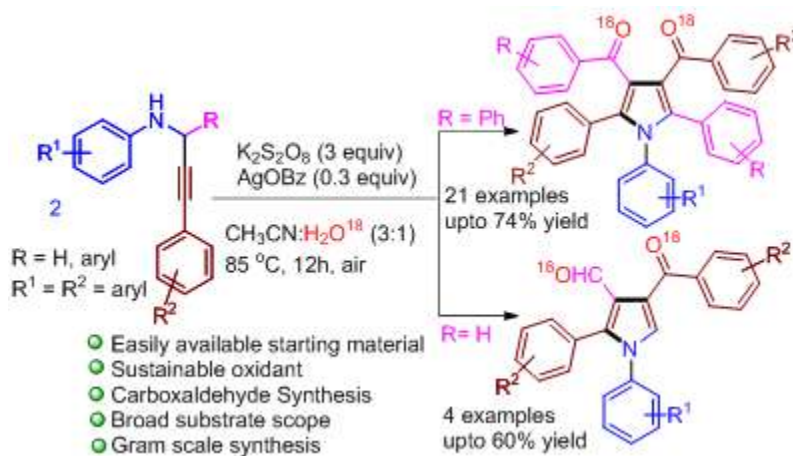
K₂S₂O₈-mediated Synthesis of Highly Functionalized Pyrroles via Oxidative Self-dimerization of *N*-Propargylamines

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Highly Substituted Pyrroles is an important structural motif also encountered in some biologically active molecules.¹An efficient methodology has been developed for the synthesis of tetra- and penta-substituted pyrroles via oxidative self-dimerization of *N*-propargylamines catalyzed by silver benzoate in presence of K₂S₂O₈ in good yields. The protocol provides a simple route for the synthesis of both tetra- and penta-substituted pyrroles with two carbonyl groups in the side chain. The methodology can be extended towards the synthesis of pyrrolo[3,4-*d*]pyridazine.



Scheme 1

References:

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Engineering of β -turn mimetic models using short azapeptides: understanding the role of $N_{amide} \cdots H-N_{amide}$ hydrogen bond in their stability

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Over the recent years, attention have been increasing towards the Azapeptides as a peptidomimetics, in which the α -carbon atom of one or more amino acid residues in a peptide chain are isosterically replaced with nitrogen atoms. Azapeptide models show improved cell-permeability and enhanced proteolytic stability compared to their peptide counterparts.¹ Azapeptides are reported to be conformationally rigid and the conformational behaviours of azapeptides are explained by the lone pair – lone pair repulsion of the adjacent nitrogen atoms. Short azapeptide are known to form β -turn types of structure, which is one of the frequently abundant secondary protein structures.² Usually, β -turns are stabilized by the presence of conventional $C=O \cdots H-N$ hydrogen bond between i^{th} and $(i+3)^{\text{th}}$ residues and $CO \cdots CO \rightarrow \pi^*$ interactions.

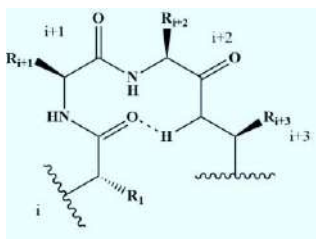


Fig1: Peptide β -turn

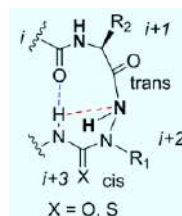


Fig2: Azapeptide β -turn models

Recently, our research group has reported an unusual $N_{amide} \cdots H-N_{amide}$ hydrogen bond in azapeptide and N-methyl azapeptide model systems, which also shows the possibility in stabilizing azapeptide β -turn like structures.³ In continuation to this work, we propose a new pathway for engineering β -turn mimetic system using N-methylated Proline and Valine based azapeptides. The role of the recently discovered unusual $N_{amide} \cdots H-N_{amide}$ hydrogen bond in stabilizing azapeptide β -turn are explicitly studied by both theoretical and experimental methods.

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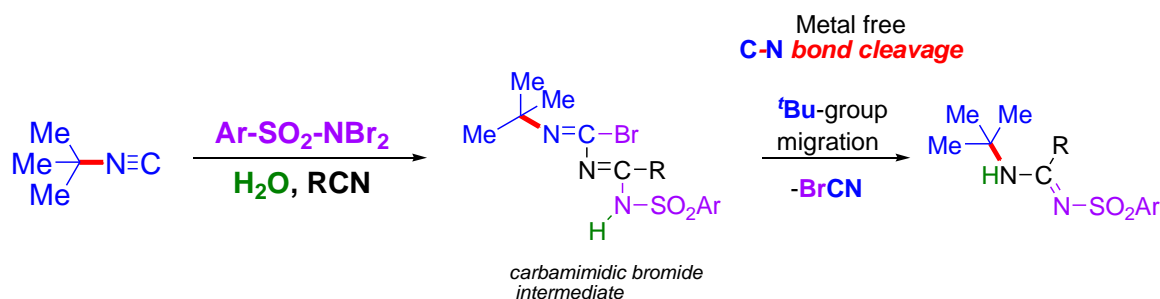
Unprecedented 1,3-*tert*-Butyl migration via C-N single bond scission of isonitrile: An expedient metal-free route to *N*-sulfonylamidines

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An unprecedented 1,3-migration of *tert*-butyl group was observed while reacting *tert*-butyl isonitrile with *N,N*-dibromoaryl sulfonamides and nitrile. The reaction involves simultaneous C-N single bond scission of isonitrile and migration of the *tert*-alkyl group to adjacent unsaturated nitrogen centre of the nitrile precursor which eventually results in the formation of *N*-sulfonylamidine. Formation of a carbamimidic bromide species at the intermediate stage of the reaction has been speculated which was confirmed by LC-MS study of the reaction mixture. This method constitutes a new route for sulfonylamidine which does not rely on transition metals. The protocol exhibits significant advantage in terms of substrates scope and additionally offers easy synthesis of guanidine molecules.



Scheme: Synthesis of sulfonylamidines

Reference:

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***Phyllanthus niruri*. L prevents palmitate induced insulin resistance condition in muscle cells via SIRT1/AKT pathway**

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Type 2 diabetes (T2D), formerly known as adult-onset diabetes has emerged as the major worldwide epidemic of the 21st century. It is seen that western medications are frequently associated with severe adverse drug reactions and high costs of treatment. Herbal medications have long been used in the treatment and prevention of T2DM in Traditional Indian Medicine (TIM). In recent years, there has been a profound interest in the role that oxidative stress in the peripheral tissues plays to induce insulin resistance. Oxidative stress occurs when there is an imbalance of Reactive Oxygen Species (ROS) formation and reduced antioxidant defences. Insulin resistance in skeletal muscle is a major and early feature in the pathogenesis of type 2 diabetes. This pathological condition has been shown to involve decreased activity of the insulin signaling network. The study aims to focus on *Phyllanthus niruri*. L, a herbal medicinal plant for preparation of an enriched active fraction and to explore the possible mechanism of action of enriched standardized (chemically defined) fraction / bioactive compound(s) of the folklore medicinal plant using different bioassays on *invitro* (cell line) and *invivo* (rat model) conditions for treating diabetes. The methanol extract as well as ethyl acetate fraction showed increased glucose uptake in muscle cell line and significant ROS inhibition assay. It was found that the expression of SIRT1 was enhanced when treated with the ethyl acetate fraction in diseased condition (FFA induced muscle cell line). Marker compound(s) isolation and efficacy studies are under progress.

Study of the effect of traditional medicinal plants in ameliorating the relationship between gut microbiota and intestinal epithelium in preventing non-alcoholic fatty liver disease (NAFLD)

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Non-alcoholic fatty liver disease (NAFLD) is a growing epidemic in the health landscape of the modern world and needs serious attention. The multiple hit hypothesis for pathogenesis of NAFLD explains the complex interactions among genetic susceptibility variants, environmental factors, insulin resistance, and the gut microbiota. Gut dysbiosis is one of the major causes of NAFLD because of the close anatomical relationship shared by the liver and the gut. Local herbs, traditional medicines and functional foods can be an answer to the battle against gut dysbiosis mediated NAFLD. But due to limited opportunities there is a research gap in the field of traditional medicines and gut dysbiosis mediated NAFLD. A detailed study on traditional herbal therapies to tackle the global NAFLD epidemic is required which may also provide an insight in integrating herbal medicine to modern therapies. Several traditional knowledge based medicinal plants and herbs are known to work wonders in treating stomach-related ailments. These medicinal plants are a reservoir of important biologically active compounds that has potent antimicrobial, antifungal activities. These medicinal plants can be used to treat a dysbiotic gut and revert the dysbiosis into a healthy gut microflora. Thus, the traditional knowledge of medicinal plants used in stomach ailments can be incorporated in modern scientific techniques to find a cure for gut dysbiosis related NAFLD. In order to bridge the widening gap between NAFLD associated gut dysbiosis, we have developed an approach to screen several traditionally known anti-microbial plants. According to the traditional herbal healers, we have selected 13 plants consisting of *Oxalis corniculata*, *Garcinia morella*, *Centella asiatica* etc. Among the selected plants, *Garcinia morella* showed potent anti-microbial activity. *Garcinia morella* (Gaertn.) Desr. belonging to Clusiaceae family is mainly distributed in India, Sri Lanka and Southern Philippines. *Garcinia* comprises of 200 species in which almost 20 are available in India and they have been extensively used in Ayurvedic medicinal practices for treating various diseases. *Garcinia* species are well endowed with secondary metabolites and hence exhibit various activities such as antibacterial, antifungal, anti-inflammatory, antioxidative and anticancer. *Garcinia morella* Desr., fruit locally known as kujithekera, is used as home remedy for stomach ailments, inflammatory disorders and gastritis. Despite its rich traditional uses, not much scientific study on NAFLD associated gut dysbiosis has been undertaken for this plant species. (Choudhury, B., Kandimalla, R., Elancheran, R., Bharali, R., & Kotoky, J. (2018). *Garcinia morella* fruit, a promising source of antioxidant and anti-inflammatory agents induces breast cancer cell death via triggering apoptotic pathway. *Biomedicine & Pharmacotherapy*, 103, 562–573. doi:10.1016/j.biopha.2018.04.068). In order to check the efficacy of *Garcinia morella* in preventing intestinal disruption, *in vitro* experiments were carried out using CaCo-2 as a model for intestinal epithelium. In this experiment, opportunistic pathogens were used as stimuli for induction of intestinal epithelial disruption. The treatment of polarized epithelial cells with opportunistic pathogens decreased the transepithelial resistance (TER) of polarized CaCo-2 cell monolayers, measured using Millicell-ERS-II Volt Ohm meter (Millipore Corp.). It was observed that simultaneous treatment of polarized epithelial cells with *Garcinia morella* extract along with opportunistic pathogen attenuated the decrease in TER of polarized CaCo2 cell monolayers. Therefore, the *Garcinia morella* extract showed promising results in the preliminary *in-vitro* experiments in prevention of intestinal epithelial layer disruption and further *in-vitro* as well as *in-vivo* studies will be carried out to confirm the potential of *Garcinia morella* extract in treating gut dysbiosis mediated NAFLD.

REMOVAL OF METHYLENE BLUE FROM AQUEOUS SOLUTION USING GROUND NUT SHELL

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Methylene blue is one of the commonly used dye, which is used in number of fields such as dyeing cotton, detecting oxidizing agents, staining tissue samples, etc. It is a water soluble cationic dye. The presence of dyes in effluents is a major concern due to their adverse effects to many forms of life. The discharge of dyes in the environment is a matter of concern for both toxicological and esthetical reasons. The present study is based on the removal of methylene blue using low cost adsorbent such as ground nut shell powder(GNSP). Ground nut shell was collected from the local market and was washed several times. The shells were then dried and grinded to form powder. This powder is sieved to particle sizes 40,63,75, 90 and 125 micron and stored in plastic bottle for use as an adsorbent. The batch adsorption was carried out to find the adsorption capacity of GNSP from aqueous solution. The effect of various parameters viz. effect of agitation time and effect of adsorbent size on the adsorption of methylene blue have been studied. Effect of agitation time reveals that adsorption was maximum in first 15 minutes, i.e. 96.32%.The equilibrium time was found to be 30 minutes for GNSP. The high adsorption at initial stage is due to the larger number of adsorption sites available which decreases with time as the number of available sites gradually decreases. Effect of adsorbent size reveals that adsorbent size increases the %removal of methylene blue also increases.This is because the pore size becomes larger enough to adsorb the methylene blue.The highest removal is observed for 125 micron size which is 97.99 %.The adsorption isotherm data fits Langmuir, and Freundlich isotherm well. Methylene blue from aqueous solution was successfully removed by GNSP.

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Development of Glucose oxidase based visual Biosensor using natural products for glucose detection in the application for food and liquor industry

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Gauhati University

Enzyme Glucose oxidase (GOx) is a remarkable discovery in the field of biotechnology as a biocatalyst. GOx has been widely accepted in diverse sectors owing to their ease of production, substrate specificity and green chemistry. The world's biotechnological industries currently working on the enhancement in enzyme productivity and development of techniques for increasing their stability. One of such technique is self life, for example enzyme immobilization technique. Immobilization of enzyme is defined as the imprisonment of enzyme in a distinct support or matrix. The support or matrix on which the enzymes are immobilized allows the exchange of medium containing substrate or inhibitor molecules. The matrix on which the particular enzyme GOx is immobilized, allows the exchange of medium containing substrate. There are a wide variety of matrixes available for immobilization. One of the uses of these immobilized enzymes is for development of biosensors. GOx is a very important enzyme for detection of glucose and can be used for development of glucose biosensor while immobilized. We are working on the fabrication and characterization of Glucose biosensor using GOx. GOx is widely used for the determination of free glucose in body fluids which has many importances in the clinical industry. There are many challenges for the development of the glucose sensor. To overcome these challenges, nanomaterial (CNTs, graphene) based biosensors are developed due to their more surface area, high biocompatibility, and efficient electrical conductivity. And the wide use of synthetic/chemical matrices for the immobilization of glucose biosensor will cause harm environment as these synthetic materials are not biodegradable. Here in this study, we have used all the natural substances as matrices such as pomelo, coconut fiber, onion inner membrane, egg shell inner membrane, sugarcane fiber and *Luffa cylindrica* (Bhol in assamese), which are very easily available, biodegradable which causes no harm to the environment, and are cost effective too. We have determined the shelf life of these natural matrices for the immobilization of the enzyme GOx. And also we determined are these natural substances worth using for fabrication of GOx biosensor. We have used the cross linking method for immobilization of GOx. For cross linking nafion is used as it helps in cross linking of the matrix with the enzyme and help the enzyme to bind properly to matrices. Immobilizing GOx enzyme on the pomelo, coconut fiber, onion inner membrane, egg shell inner membrane, sugarcane fiber and *Luffa cylindrica* matrices, we found that *Luffa cylindrica* showed highest activity with sugarcane juice substrate at a p^H of 8.5 and lowest activity with glucose substrate at a p^H of 6, coconut fiber showed highest activity on sugarcane juice substrate at a p^H of 7.5 and lowest activity with glucose substrate at a p^H of 6, onion inner layer showed highest activity on sugarcane juice substrate at a p^H of 7.5 and lowest activity with glucose substrate at a p^H of 6, egg shell inner membrane showed highest activity with sugarcane juice substrate at a p^H of 8.5 and lowest activity with glucose substrate at p^H 6, pomelo showed highest activity with sugarcane juice at a p^H of 6 and 6.5 and lowest activity with glucose at a p^H of 6.5 and sugarcane fiber matrix showed highest activity with sugarcane juice at a p^H of 8.5 and lowest activity with glucose at a p^H of 8. From the study we can conclude that matrices shows highest stability at higher p^H and lower substrate concentration. The stability of the GO_x immobilized matrix were investigated for a period of six hours and it showed reliable response while using glucose as substrate. Also we have developed a color changing visual glucose biosensor with the immobilized GOx enzyme, which changes its color from blue to colorless in presence of glucose. This color changing indicates the presence of glucose in a sample.

Leach-Resistant Support for the Fabrication of Pd⁰ Nanocatalyst for Base-free Chemoselective Transfer Hydrogenation of Styrene

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The functionalization of mesoporous SBA-15 with propylamine moiety made the material capable of scavenging Pd²⁺ ions from acetone very efficiently and the monodispersed surface bound Pd⁰ NPs were generated using NaBH₄ in water. The as-synthesized SBA-15-*pr*-NH₂.Pd⁰ nano hybrid material act as highly active, leach-resistant and recyclable heterogeneous catalyst for base-free chemoselective transfer hydrogenation of styrene to ethylbenzene using formic acid as non toxic, clean hydrogen source at 298 K temperature. The catalyst exhibited excellent performance when some substituted styrene and other unsaturated compounds having carbon carbon double bonds are employed as substrates in the optimized reaction condition for styrene. The role of free propylamine was found to be very crucial for higher conversion and selectivity of the desired alkane products.

Key words: SBA-15, functionalization, scavenging, Pd⁰ nanoparticles, styrene, base-free transfer hydrogenation.

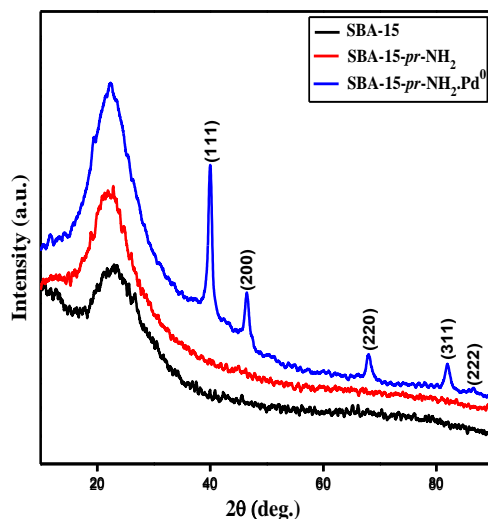


Figure: PXRD patterns of SBA-15, SBA-15-*pr*-NH₂ and SBA-15-*pr*-NH₂.Pd⁰

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Anti-diabetic effect of *Osbeckia nepalensis* Hook. in modulating hepatic gluconeogenesis through AMPK dependent inhibition of gluconeogenic enzymes

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Liver is the largest organ in the human body and maintains the glucose balance in the body through different pathways like glycolysis (breakdown of glucose), glycogenolysis (breakdown of glycogen) and gluconeogenesis (glucose production from non-carbohydrate substrates). But due to the rise in trends of improper food habits and less physical activities in the modern day world, certain conditions disrupt the normal glucose homeostasis pathway leading to increase in obesity as well as enhanced glucose production. Abnormal enhanced glucose production in liver due to high circulating free fatty acids (FFA) leads to hyperglycemia, which is one of the main markers of type 2 diabetes mellitus in both old as well as young adults. A protein kinase, AMP activated protein kinase (AMPK) also regulates glucose homeostasis by inhibiting the gluconeogenic genes through insulin independent pathway. According to International Diabetes Federation 2019, there are 463 million people worldwide living with diabetes and is expected rise by 700million and T2DM accounts for 90% of all the diabetes cases. Several drugs like metformin, a highly circulating drug to reduce hyperglycemia, is being prescribed as one of the anti-diabetic drugs to the patients but it is not metabolised in liver and also causes several side effects like renal toxicity, nausea, hypoglycemia, etc. So, natural product based anti-diabetic drug development, with no side effects, is one of the major challenges among the researchers. Based on the traditional knowledge gained from the traditional herbal healers of North East India, we have selected *Osbeckia nepalensis* Hook. an edible medicinal plant (Melastomataceae) for the study of its effect in downregulating the hepatic production of glucose. The crude extract along with its fractions and sub fractions as well as isolated compounds are found to be effective in the uptake and utilization of glucose in *in vitro* conditions. It was also found that the expression of activated AMPK was enhanced along with the downregulation of gluconeogenic enzyme, phosphoenol pyruvate carboxykinase, PEPCK, and the rate limiting enzyme, glucose 6 phosphatase, G6P, when treated with the plant extracts in diseased condition (which is achieved by the treatment of palmitate on primary hepatocyte cells). Therefore, the enriched chemically defined fraction of *Osbeckia nepalensis* Hook. may be used as dietary supplement to control the excess hepatic glucose production in T2DM patients.

Film-Based Electronic Volatile Acid Vapor Sensor with Ultrahigh Sensitivity for Real-Time Analysis

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Global industrialization leads to the discharge of harmful volatile acid vapors into the environment, causing damage to various forms of life. Therefore, the development of rapid sensing systems for monitoring of volatile acid vapors is of significance for a safe and clean environment. Herein, the properties of a conjugated organic moiety combined with a commercial economic polymer to obtain composite film are designed for the selective detection of volatile acid vapor, viz., hydrogen chloride. The excellent electrical behavior of the obtained film thus allows its efficient use as a smart sensor film for the detection of hydrogen chloride vapors with quick response, reversibility, and selectivity with a low detection limit of 9 ppb. Taking advantage of this remarkable behavior in response to acid vapors, we have designed an electronic prototype for on-field applications with visual detection of hydrogen chloride vapors in ambient conditions. Compared to the other exploited approaches for hydrogen chloride detection, the polymer-supported active-film-based prototype is simple, portable, and cost-effective and can be used for real-time monitoring.

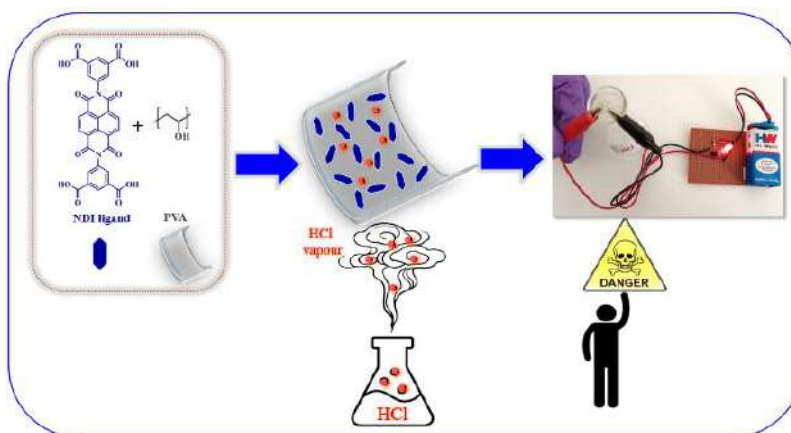


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Synthesis of *N*-(pyridin-2-yl)anthracene-9-carboxamide and its application as fluorescent “turn-on” sensor for Hg(II) ion

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A new compound *N*-(pyridin-2-yl)anthracene-2-carboxamide has been synthesized and its turn on fluorescence sensing property towards various metal ions have been studied. Further, we observed that the compound was highly sensitive towards Hg²⁺ ion in solution. We have also done the theoretical study for the compound synthesized by using DFT method and Gaussian 09 series of program. The compound was characterized by FT-IR, NMR and single crystal XRD. [1-4]

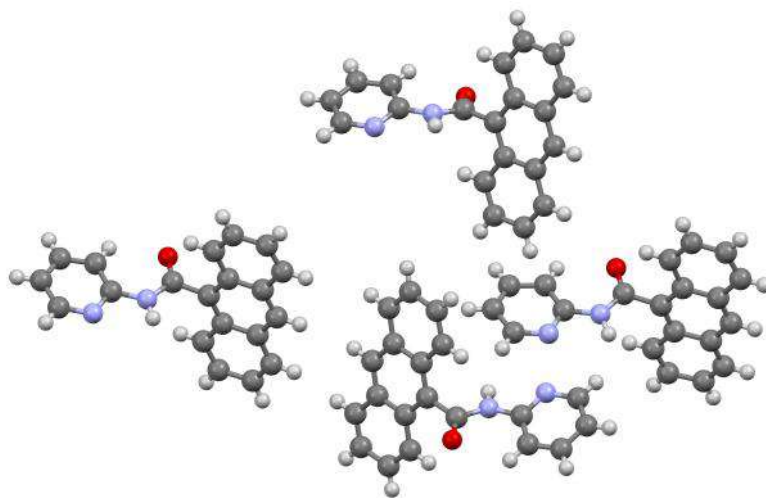


Figure:Single crystal XRD structure of the *N*-(pyridin-2-yl)anthracene-2-carboxamide

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Binding Interaction of a Potential Statin with β -lactoglobulin: An In Silico Approach

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This study reports the interaction between a synthetic statin, Fluvastatin with bovine milk protein, β -lactoglobulin (BLG) [1] through docking, molecular dynamics simulation (MD) and binding free energy calculations. Docking provides the best fitted binding mode of the ligand with the receptor. We have carried out MD simulations of the protein and protein-ligand complex at two different pH viz. 7.0 and 1.5 [2]. We have found that the protein shows more compact behaviour at pH 1.5 and this behaviour is more prominent on complexation with the ligand. Calculations of hydrogen bonds at pH 1.5 confirms that hydrogen bonding interactions of the binding residues of the protein with the ligand provides stability to the complex. MM-GBSA calculations suggest that there is favourable binding interactions between the protein and the ligand with major contributions from Vander Waals interactions. This study suggests that in spite of the acidic environment in the stomach BLG can act as a carrier for the acid-sensitive drug molecules because of its highly stable behaviour in the acidic pH.

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Heteroleptic Copper(II) complexes of 1,10-Phenanthroline with S-methyldithiocarbazate based Schiff base Ligands: Synthesis, Structure, Spectral and Redox properties

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A series of copper(II) complexes of the types $[\text{Cu}(\text{L})(\text{phen})](\text{ClO}_4)$ **1-4**, where HL is a tridentate ligand with two nitrogen and one sulphur donor atoms (NNS) such as N'-pyridin-2-ylmethylene-hydrazinecarbodithioic acid methyl ester (HL1) N'-(1-pyridin-2-yl-ethylidene)-hydrazinecarbodithioic acid methyl ester (HL2), N'-quinolin-2-ylmethylene-hydrazinecarbodithioic acid methyl ester (HL3) and N'-(1-methyl-1H-imidazol-2-ylmethylene)-hydrazinecarbodithioic acid methyl ester (HL4), phen is 1,10-phenanthroline. The ligands and its complexes were characterized by physicochemical techniques, viz., molar conductance, cyclic voltammetry, IR, NMR, EPR, UV-Vis spectroscopy and mass spectroscopic techniques. The crystal structure of all the compounds was also characterized by single crystal X-ray crystallography. The SCXRD studies reveal the structure of the complexes intermediate between square pyramidal distorted trigonalbipyramidal (SPDTBP) and trigonalbipyramidal distorted square pyramidal (TBDSP) geometry. Dithiocarbazate moiety binds with copper atom in a deprotonated form via thiolate S atom, azomethine N atom and the N atom of pyridine of tridentate dithiocarbazate moiety in NNS fashion where as other two sites are occupied by two nitrogen atoms of co-ligand phenanthroline. Non-bonded perchlorate anion is found outside the coordination sphere which neutralise unipositive copper complexes. In this present work we try to investigate the chelating properties of the ligands which have great impact on promising biological implications, structural diversity, ion sensing ability and catalytic activities.

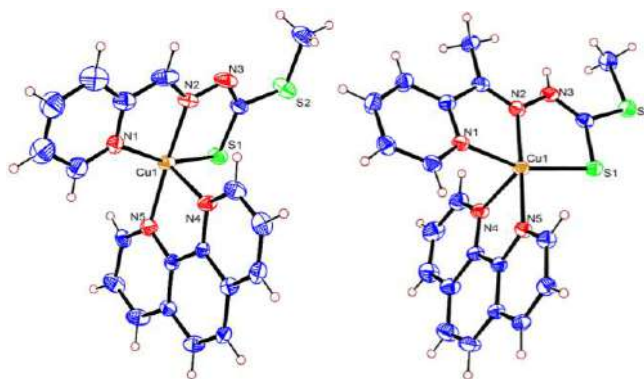


Figure 1. ORTEP diagram of the Cu(II) complexes **1** and **2** with ellipsoids at the 30% probability level. Perchlorate anion and solvent molecules are omitted for clarity.

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- 2.

Utilization of Advanced Oxidation Process for the Treatment of Formation Water

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The oil-field formation water is the wastewater generated during oil and gas exploration activities in various parts of the globe. Formation water mainly contains a large amount of organic and inorganic loads and responsible for polluting the nearby areas of the crude oil drilling site. This has emerged as a significant environmental problem. One of the most challenging issues of the last few decades is the removal of various contaminants present in the oilfield formation water. This study is aimed at the treatment of oilfield formation water using Advanced Oxidation Processes (AOPs). In this work, AOP was carried out at a pH of 3-8, and higher efficiency of hydrocarbon degradation was observed at pH near about 3 and 4. It was observed that AOP could effectively remove more than 85% of the organic matter from the formation water sample (Figure 1). Samples were analyzed by Gas Chromatography-Mass Spectroscopy (GCMS) to estimate the level of contamination.

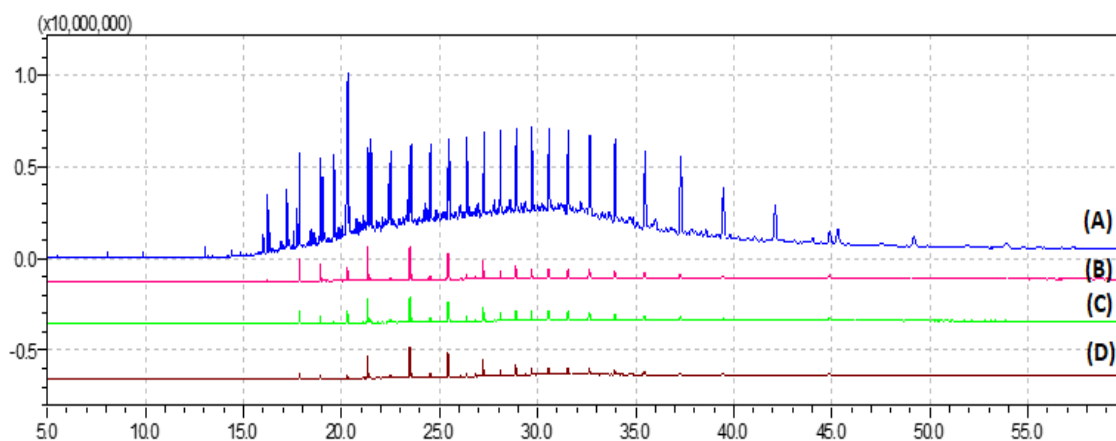


Figure: Comparative GCMS Chromatogram for control and test samples .A: Control (Untreated sample), B: Treated with AOP (without adjusting the pH), C: Treated using AOP (at pH 3), and D: Treated with AOP (at pH 3 and Temp. 45°C).

Influence of non-covalent interactions in dictating the polarity and mobility of charge carriers in a series of crystalline NDIs: A computational case study

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Polycyclic aromatic compounds and their derivatives have emerged as potential molecular entities for air-stable *n*-type organic semiconductors. Especially, naphthalene diimide (NDI) derived compounds stand out as one of the most promising class of molecules that have been studied extensively. There has been a lot of debatable experimental reports on the OFET performance characteristics of some of these materials which are not yet been resolved completely. Hence, the critical intrinsic aspect of the molecular materials on the charge transport in bulk crystalline state would be essential to categorise the potential candidates. As a case study, in this comprehensive computational approach, we have investigated the structural and supramolecular organization in single crystals and the role of those aspects on the bulk carrier transport of a group of selected end-substituted NDI derivatives. A subtle alteration of the end group is observed to result in modulating the polarity of charge transport and the charge carrier mobility in the single crystalline state. The disparity is addressed by considering the electronic coupling of the transport states, symmetry of the frontier molecular orbitals and various non-covalent intermolecular interactions. We expect that the present study would benefit towards rational designing of the air-stable *n*-type organic molecular semiconductor for efficient electronic devices.



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Antioxidant and physicochemical study of Chitosan/poly(ethylene glycol) based biocomposite films using natural extract as an active component

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In this study, the effects of incorporation of natural extract on the antioxidant activity and physicochemical properties of chitosan and poly(ethylene glycol) blend films were evaluated. The prepared films were examined for antioxidant and physicochemical properties. The antioxidant activity of the films was studied via DPPH (2,2-diphenyl-1-picrylhydrazyl) free radical scavenging assay. The mechanical properties of the films decreased marginally with the incorporation of the plant extract. However, incorporation of the plant extract in the films significantly decreased the water content, solubility and swelling of the films which is considered as a favourable property of packaging films. The UV-visible light blocking properties increased with the incorporation of the plant extract. The findings of the study established the prepared films as suitable material for food packaging. These eco-friendly prepared films are cost effective and may be used as an active food packaging material.

Keywords: Chitosan, poly(ethylene glycol), thin-film, food packaging, natural extract

Chaotropic Effect of ions on the Self-Aggregating Propensity of Whitlock's Caffeine Molecular Tweezers: A Molecular Dynamics Study

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Molecular Tweezers, feature the first class of artificial receptors to have long fascinated researchers and emerge as an efficient drug candidate from a supramolecular host with outstanding results in animals. The tweezers being endowed with exceptional structure and excellent selectivity, very well complex to guest moieties through various non-covalent interactions. Their exquisite binding specificity, by altering the cavity depending on the guest-configuration, nature and flexibility of the spacer-unit, establishes this overall class of receptors as a promising tool, with abundant applications to biology and medicine. However, the tweezers' inclination to self-aggregate by mutual π - π stacking interactions of their flat, extended aromatic arms, diminishes their efficacy as a therapeutic candidate. Therefore, following up on sporadic studies, since the discovery of the Hofmeister series, regarding the ability of ions to either solvate (salting-in) or induce aggregation (salting-out) of hydrophobic solutes, we utilised the notions of ion-specificity effects on tweezer moieties. We investigated the impact of electrolytes containing trivalent aluminium cations bearing three different anions, viz. Cl^- , ClO_4^- and SCN^- on the self-association propensity of caffeine-pincer molecular tweezers. The Hofmeister series was validated, with specific emphasis placed on elucidating the varied behaviour of the electrolytes on the tweezers' hydration ability. We conducted a comparative investigation, employing a series of all-atom molecular dynamics simulations to gain a clear grasp of how such aggregation might be prevented. We observe a steady reduction in the aggregation tendency and an increase in the salting-in behavior of the receptor molecules, as we progress along the Hofmeister salt solutions, from AlCl_3 , $\text{Al}(\text{ClO}_4)_3$ to $\text{Al}(\text{SCN})_3$. Radial distribution functions, average hydrogen bond analysis, contour maps, solvent accessible surface area values showed that, ions altered the solubility of the extended tweezer molecules by altering their overall water structure. Cl^- being the most charge-dense of the three anionic species, was seen to experience stronger hydration, therefore, being excluded from the vicinity of the hydrophobic tweezer molecules. This resulted in an increase in the water densities around the tweezer leading to higher aggregation. While, ClO_4^- and SCN^- ions being less charge-dense were poorly hydrated and hence, behaved more like hydrophobic solutes. SCN^- ions exhibited the highest interaction with the tweezer molecules and thereby, displayed the greatest salting-in ability. The results obtained were further validated by the interaction parameter values and cluster structure analyses.

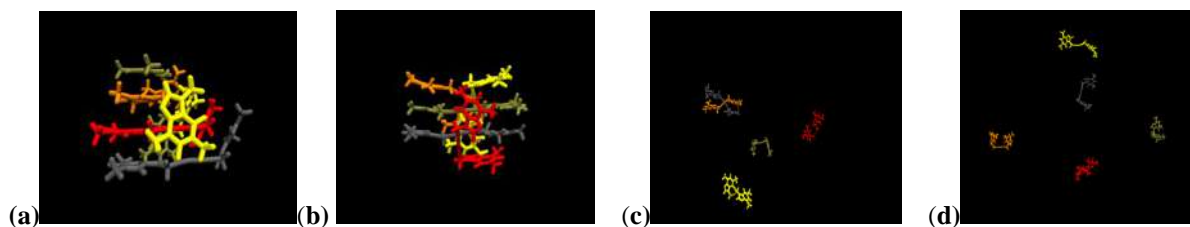


Figure 1. Snapshots of five caffeine-pincer molecular tweezers captured after 300 ns simulation run (a) pure water system, (b) AlCl_3 system, (c) $\text{Al}(\text{ClO}_4)_3$ system and (d) $\text{Al}(\text{SCN})_3$ system.

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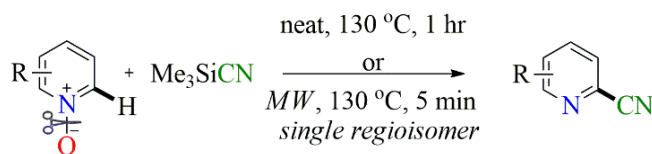
Regioselective Cyanation of Six-Membered *N*-Heteroaromatic Compounds Under Metal-, Activator-, Base- and Solvent-Free Conditions

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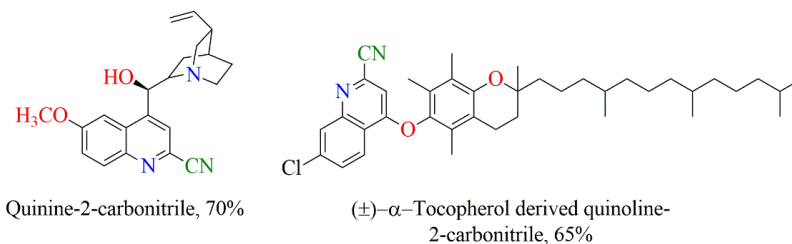
2-Cyano heterocyclic scaffolds are a prominent class of synthetic intermediates, which have found application in the preparation of a wide variety of bio relevant compounds and pharmaceuticals. To date, a number of synthetic protocols were developed with metal, base and activating agent. However, all of these bear their own limitations, such as lack of regioselectivity, required super-stoichiometric amount of base, toxic, hazardous, air and moisture sensitive reagents used as activator and use of hazardous halogenated solvents. Herein, we report a simple, one-pot method for the C-H cyanation of heteroarenes *N*-oxides with trimethylsilyl cyanide which proceeds smoothly in conventional heating and also under microwave irradiation with shorter reaction times under metal-, activator-, base- and solvent- free conditions. The present protocol is applicable to broad range of substrates with good chemoselectivity and regioselectivity. The synthetic utility of C2-substituted heteroaromatic nitriles is widely explored into several bio-active molecules including late-stage functionalization of anti-malarial drug quinine, and (±)- α -tocopherol modified quinoline derivative. Based on experimental studies, a plausible mechanism is put forward involving dual role of trimethylsilyl cyanide as cyanide source as well as activating agent.



Scheme: C2-cyanation of *N*-heteroarene-1-oxides with trimethylsilyl cyanide

√ Metal-, activator-, base- and solvent free√
Excellent regio- and chemo-selectivity

√ Broad substrate scope, scale-up
√ aqueous work up, yields upto 98%



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Multifunctional N-doped Carbon Dots for Bimodal Detection of Bilirubin and Vitamin B₁₂, Living Cell Imaging, and Fluorescent Ink

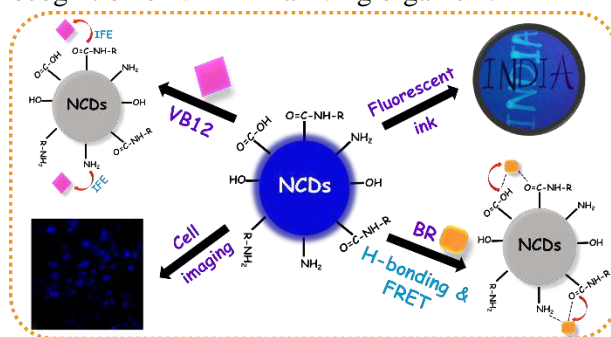
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A N-doped carbon dot (NCDs) has been synthesized via a simplistic one-step hydrothermal technique using L-aspartic acid and 3,6-diaminoacridine hydrochloride. The NCDs exhibit a high quantum yield (22.7 %) and excellent optical stability in aqueous media. Additionally, NCDs display good solid-state yellowish-green emission and are suitable for security ink applications. The remarkable fluorescence (FL) properties of NCDs were further applied to develop a multifunctional sensor for bilirubin (BR) and vitamin B₁₂ (VB12) via fluorescence quenching. We have systematically studied the FL quenching mechanisms for the two analytes. The primary quenching mechanism of BR was via the FRET pathway facilitated by the H-bonding network between the hydrophilic moieties existing at the surface of BR and NCDs. In contrast, IFE was mainly responsible for the recognition of VB12. The practicability of the nanoprobe NCDs was further tested in real samples analysis for BR (human serum and urine samples) and VB12 (VB12 tablets, human serum, and energy drink) with a satisfactory outcome. The *in vitro* competency was also verified in the human cervical cancer cell line (HeLa cell) with negligible cytotoxicity and significant biocompatibility. This result facilitates the application of NCDs for bioimaging and recognition of VB12 in a living organism.



Scheme. Blue-emitting N-doped carbon dot for highly selective and sensitive detection of bilirubin & vitamin-B₁₂, living cell imaging and fluorescent ink.

Photocytotoxic Co(II) complexes having an anthracene-based curcuminoid ligand

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The current surge in the design of cytotoxic agents for cancer treatment that act through novel mode of action has stimulated extensive research in the field of photo-activated chemotherapy (PACT).^{1,2} The ability to coordinate various organic compounds of choice to transition metals and their tuneable redox activity give immense opportunities to design and develop such diagnostic/therapeutic agents.^{3,4} Herein, we present the synthesis, characterization and *in vitro* photocytotoxicity study of four Co(II) complexes *viz.* [Co(L₁)(L₂)₂](OAc)(**1-4**) where, L₁=1,7-(di-9-anthracene-1,6-heptadiene-3,5-dione)(9-accm)(**1, 2**), 1,3-Diphenyl-1,3-propanedione(dibenzoylmethane, dbm) (**3, 4**) and L₂=1,10-phenanthroline(phen)(**1, 3**), dipyrido[3,2-a:2',3'-c]phenazine(dppz)(**2, 4**).⁵ All the prepared complexes were characterised by UV-Vis, FT-IR, elemental analysis, fluorescence spectroscopy, cyclic voltammetry and magnetic susceptibility measurements. They were found to have moderate binding propensity for human serum albumin (HSA) and calf thymus (*ct*-DNA) which indicate their potential biological application. The complexes show prodigious photo-enhanced cytotoxicity in human cervical cancer (HeLa) and breast cancer (MCF-7 and MDA-MB-231) cells with low dark toxicity. From DAPI staining, AO/EB dual staining and Annexin-V-FITC experiments, it's cleared that complexes induce cell death primarily *via* apoptotic mechanism in HeLa cells.

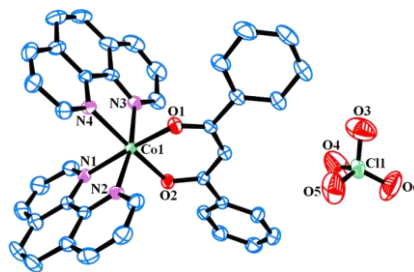


Fig: Single Crystal X-Ray Diffraction Structure of Complex **3**

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Perovskite : The Future Generation Photovoltaics

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The solar energy is a non-vanishing renewable source of energy which is pollution free. It has the potential to become the alternative source of clean energy replacing non-renewable energy comprising fossil fuels and petroleum deposits found inside earth. The fabrication of solar cells has passed through a large number of improving steps from one generation to another. Starting from the era of Cesar Becquerel, Charles Fritts solar cell has made a magnificent improvement and many new types of solar cells have been developed over the years. Among different types of solar cells, perovskite solar cells (PSCs) are the most emerging area of research among different new generation photovoltaic technologies due to its super power conversion efficiency (PCE). Among different types of solar cells, perovskite solar cells (PSCs) have drawn significant attention of researchers from both academia and industry. Perovskite solar cells (PSCs) have been of interest to Scientists receiving considerable attention in recent years as a promising material capable of developing high performance photovoltaic devices at low cost. However, significant barriers remain standing in the pathway of PSC advancement. The development of high-efficiency, stable devices and environment benignant perovskites is critical, yet challenging aspects remain in PSC research. This presentation emphasis on the recent advances in related subjects. The approaches for high power conversion efficiency, instability issues and changes on malignant component of perovskites have been discussed.

Keywords: fossil fuel, barrier, photovoltaic, perovskite, benignant.

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Isolated compounds from *Leucaena leucocephala* (Wild Tamarind) attenuate oxidative stress related to type II diabetes mellitus via modulation of SIRT1/AKT signalling pathway

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In today's world where stress and busy lifestyle are two major components for all, metabolic conditions related diseases like type 2 diabetes is increasing in a scary rate. One of the various factors that contribute to development of chronic diabetic complications is oxidative stress. Oxidative stress is generated by an imbalance between the rate of reactive oxygen species generation (ROS) and the antioxidant defence systems of the body. Oxidative stress is a major upstream event for development of insulin resistance through initiating a cascade of deleterious pathophysiological mechanisms leading to Diabetes mellitus. Natural products as drug lead have always been an attractive field of therapeutic breakthrough. Besides ever-increasing demand of nature based/ nature mimicking ways of treatments for various ailments and also the side effects of the commonly used drugs pushed the traditional medicine system (T&CM) into picture, with its lesser side effects, age old use in dietary system and comparatively easy access.

Leucaena leucocephala (Lamk.), a tropical tree species, was known as "miracle tree" in the 1970s and early 1980s, because of its highly nutritious values worldwide. Although many phytochemicals have been reported from the plant proper scientific studies relating its photochemistry and bioactivity effects are still limited. In a previous study reported by our group the plant was found to be having significant antidiabetic potential in a preliminary enzymatic investigation. In this study, the antioxidant and ROS inhibiting potential of the young seeds of *L. leucocephala* has been observed from *invitro* antioxidant assays. Immunoblotting experiments suggested that the antidiabetic potential of the plant is through the modulation of SIRT1/AKT signalling pathway. Phytochemical investigations of the plant resulted in the isolation of five bioactive/marker compounds, identification/structure elucidation of which are under process. Figure 1 below shows the HPLC chromatograms of the crude plant extract and that of the isolated compounds. Figure 2 are predicting the antihyperglycemic activity of the plant extract and its active fraction (Ethyl acetate fraction) through the positive glucose uptake result in C2C12 myoblast cell.

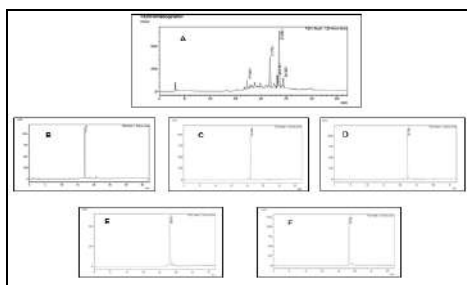


Figure 1: HPLC chromatogram of A) *Leucaena leucocephala* crude extract and its isolated molecules 1 (B), 2 (C), 3 (D), 4 (E) and 5 (F)

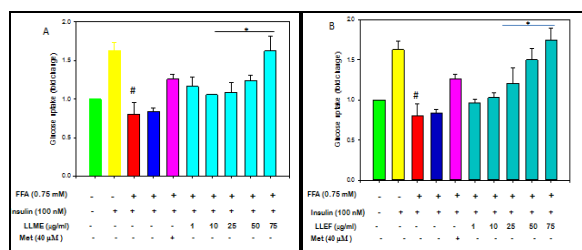


Figure 2: Effect of the A) *Leucaena leucocephala* crude extract and B) *Leucaena leucocephala* ethyl acetate fraction on Glucose uptake in palmitate (PA) treated C2C12 cells. Cells were pre-treated with drug in different micro molar concentrations (1-75 µg/mL) for 2 h followed by PA (0.75 mM) exposure for the next 20 h. “#” denotes the significant difference from untreated (p#<0.05) and “*” denotes the significant difference from PA-treated groups (p* < 0.05).

Condensation Product Of Salicylaldehyde And 3-Aminophenol: A Switch-On Probe For The Fluorescent Detection Of Cerium (III)

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Cerium is a significant lanthanide and one of the most abundant rare earth elements [1-4] and cerium (III) is the most abundant type of cerium in the earth [2]. Cerium has industrial applications viz. metallurgy, glass and ceramics, lighting and television, catalytic converters in vehicles [1], polishing powder, magnets, catalysts, ceramic colorant [2]. It also has agricultural and some therapeutic applications [3]. On the other hand, cerium is hazardous since its fume inhalation cause lung embolisms, on accumulation in the body, it is detrimental to liver tissue [1], can cause sensitivity to heat, abnormal blood, acute myocardial infarction, biochemical indices, leukaemia and skin lesions [4]. Due to its wide spectrum of applications, analysing the environmental, medical and biological effects of cerium are of growing interest [1,3]. This work reports selective fluorescent detection of cerium (III) ion by a probe amongst other metal cations. Electrochemical analysis of the probe also complements its affinity towards cerium (III) ion.

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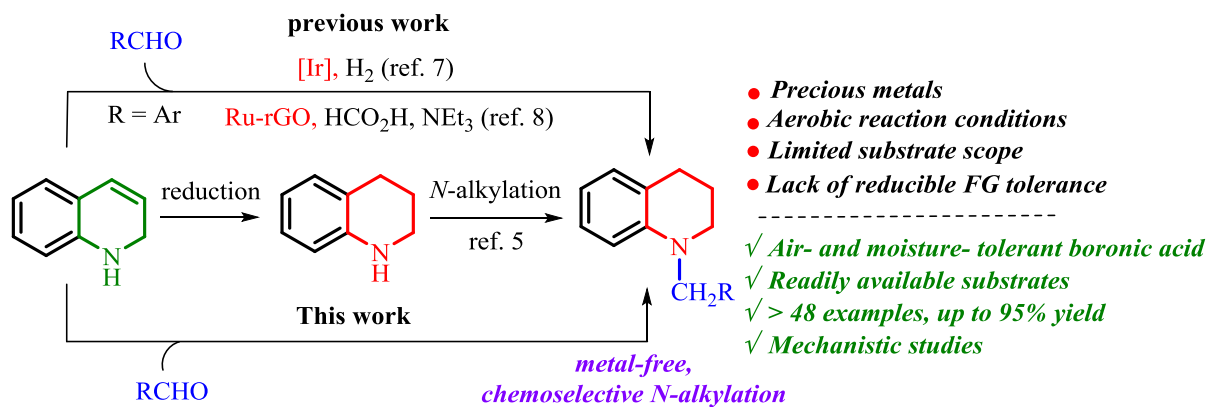
Reductive Alkylation of Quinolines to *N*-Alkyl Tetrahydroquinolines Catalyzed by Arylboronic

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A boronic acid catalyzed one-pot tandem reduction of quinolines to tetrahydroquinolines followed by reductive alkylation by the aldehyde has been demonstrated. This step-economical synthesis of *N*-alkyl tetrahydroquinolines has been achieved directly from readily available quinolines, aldehydes, and Hantzsch ester under mild reaction conditions. The mechanistic study demonstrates the unique behaviour of organoboron catalysts as both Lewis acids as well as hydrogen-bond donors.



Synthesis and Characterization of Co loaded ZSM-5/MCM-41 Composite Material from ZSM-5 zeolite

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ZSM-5/MCM-41 composite material was synthesized hydrothermally from pre-synthesized ZSM-5 zeolite with Si/Al ratio 50 as a silica source and cetyltrimethylammonium bromide (CTAB) as template. Following the same procedure, Co loaded ZSM-5/MCM-41 composite material was also synthesized by in-situ modification method using cobaltous nitrate as metal source. The synthesized composite materials can combine the advantages of both the microporous (ZSM-5) and mesoporous (MCM-41) materials such as larger pore size, high hydrothermal stability and strong acidity. The synthesized materials were characterized by FTIR, PXRD, TGA, UV-VIS DRS analysis, N₂adsorption/desorption analysis and SEM-EDAX analysis. The XRD pattern of the composite showed both the characteristic peaks of ZSM-5 and MCM-41. The incorporation of Co was confirmed by EDAX analysis. The BET surface area of the composite materials was found to be higher than that of ZSM-5 zeolite.

Key words: ZSM-5, MCM-41, Microporous, Mesoporous, Composite material.

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Protein-Activated Transformation of Non-Fluorescent Silver Nanoparticles to Blue and Red-Fluorescent Nanoclusters

P.Sarkar, D.K. Sahu, K. Sahu*

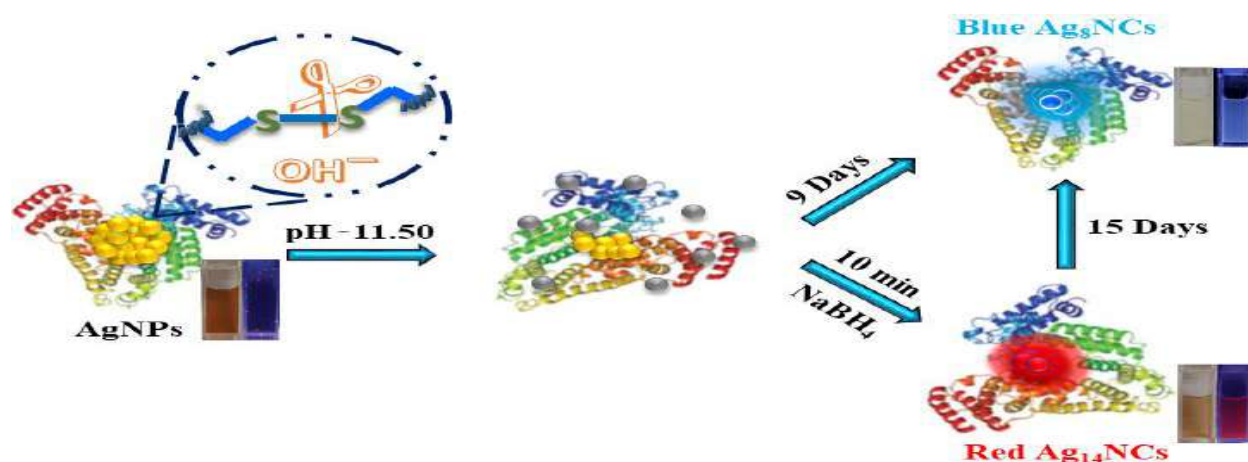
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Proteins are very effective capping agents to synthesis biocompatible metal nanomaterials *in situ*. Reduction of metal salts in the presence of protein generates very different type of nanomaterials (nanoparticle or nanocluster) at different pH. Does a simple pH jump can trigger a transformation between the nanomaterials? The concept has been materialized through conversion of silver nanoparticles (AgNPs) into highly fluorescent silver nanoclusters (AgNCs) via a pH-induced activation of bovine serum albumin (BSA) capping. The BSA-capped AgNPs, stable at neutral pH, undergo rapid dissolution upon pH jump to 11.5, followed by generation of blue-emitting Ag₈NCs under prolonged incubation (~9 days). The AgNPs can be transformed quickly (within 10 min) into red-emitting Ag₁₃NCs by adding sodium borohydride during the dissolution period. The BSA-capping is exerting both oxidizing and reducing properties in the basic solution; it first oxidizes AgNPs into Ag⁺ and then reduces the Ag⁺ ions into AgNCs.



Oxidation of Rhodamine B in aqueous medium with raw and acid-treated CoO and NiO as catalysts**Sabina Sultana and Hrishikesh Sarma****Department of Chemistry, B.Borooah College, Guwahati, Assam, India**Email: sabinakhan726@gmail.com*

Rhodamine B (RB) dye is a cationic xanthene dye widely used in the printing, textile, photographic industries and also used in foodstuff. It is harmful to humans and animals. It causes irritation of the skin, eyes and respiratory tract, and also causes carcinogenicity, reproductive and developmental toxicity, neurotoxicity and chronic toxicity towards humans and animals. It is considered as an undesirable chemical in water. In the present work commercially available metal oxides, CoO and NiO, and those activated by treating with 0.5N, 0.75N and 1.0N H₂SO₄ were used to oxidize the dye in water to innocuous compounds. The acid-treated materials showed large increases in surface area while changes in other surface characteristics were moderate in nature. The catalysts were characterized with FTIR and cation exchange capacity. Oxidation was carried out in a batch reactor at ambient temperature and pressure under different conditions of reaction time, catalyst load, reactant concentration, P^H and temperature. The result showed that conversion of Rhodamine B dye increases smoothly with increase in the reaction time from 30 to 300 min. The maximum conversion (66.6%) of RB was achieved with the catalyst 0.75N acid treated NiO catalyst. A small amount of catalyst (7.5gL⁻¹) was sufficient for maximum oxidative destruction of Rhodamine B in water. The catalysts could be recovered and reused. The kinetics of the reaction was found to be first order rate equation.

Keywords: *Rhodamine B, RB, CoO, NiO, acid treated, dye oxidation*

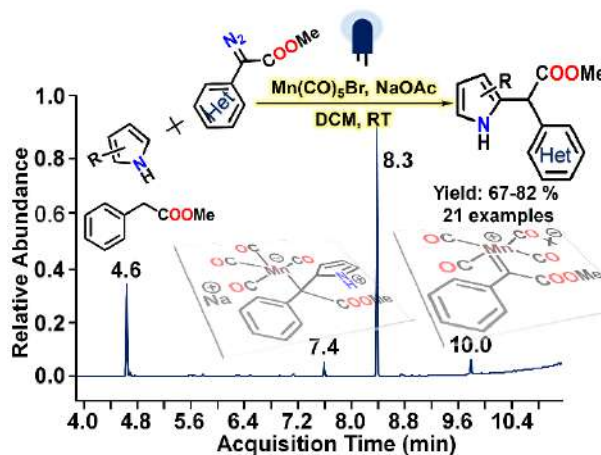
Blue LED Induced Manganese (I) Catalysed Direct C2–H Activation of Pyrroles with Aryl Diazoesters

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Transfer of carbenes from diazo moieties into many heterocycles is a useful transformation in organic synthesis.¹ This transformation involves insertion into C–X bonds (X: halides or H), addition to C–Y bonds (Y: C, N) or cyclopropanation of C=C bond. They have been utilized to modify various heterocyclic substrates such as pyrroles, indoles, furans and thiophenes. These heterocycles contain multiple reaction sites and the choice of condition including the catalyst becomes important for selective and exclusive carbene transfer reactions in these molecules. Although, there have been quite a few numbers of rhodium, ruthenium and copper catalysed carbene incorporation reactions of pyrroles by diazo compounds.² In these cases, pyrrole NH were either protected or remained free. In general, the reported carbene transfer reactions are limited in their diversity.^{1,2} Herein, in this poster, we are going to present a blue LED mediated manganese pentacarbonyl bromide [Mn(CO)₅Br] catalysed incorporation of carbene moieties from aryl diazoesters onto 1H-pyrroles via their selective C2–H activation. Along with that we will also go to discuss a detailed mechanistic pathway by which these C2–H activation takes place. During the mechanistic investigation a manganese metal-carbene species has been identified as the active catalyst to facilitate these reactions. Eighteen monosubstituted pyrrole derivatives were isolated in good to excellent yields (67 to 82%) and the disubstituted products were also formed in minor quantities (5 to 8%). HPLC based kinetics study enabled optimization of the reaction. Control experiments, FT-IR, NMR and GC-MS based characterization elucidated the putative reaction mechanism.³



Keywords: C2–H activation; pyrrole; blue LED; Mn(CO)₅Br; carbene.

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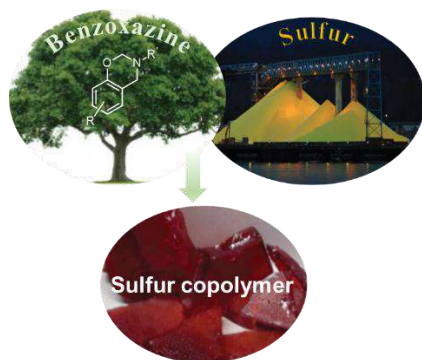
Sustainable development of copolymers made from bio based benzoxazine monomer and industrial waste sulfur

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Polymeric materials are widely produced and considered as high utility materials with wide range of applications. The major concern worldwide is their huge dependence on non-renewable petrochemical reserves. Alternative feedstocks either greener origin or waste derived needs to be explored to meet the continuous rise in demand and mitigate the environmental pollution along with sustainability. Polybenzoxazines (PBzs) are a new class of phenolic thermoset resins with high performance and tremendous applications. Several advantages associated with PBz including appreciable mechanical strength, high thermal stability, negligible water absorption, near zero cure shrinkage, ease of synthesis, catalyst free ring opening polymerization *et chas* led to their rapid advancement. In this context, copolymer synthesized from agro waste like cardanol benzoxazine (Bz) and elemental sulfur, which is a high tonnage waste generated from petrochemical industry aids to a sustainable and wide new-arena of sulfur polymeric materials. A facile method termed as “Inverse Vulcanization” will be reviewed with emphasis on the utilization of waste sulfur with organic co-monomers. These polymeric materials possess tunable thermo-mechanical, electrical and optical properties.



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Synthesis, structural studies and DFT calculations of tricarbonylrhenium(I) metal complexes containing nitrogen based N∩N donor polypyridyl ligands

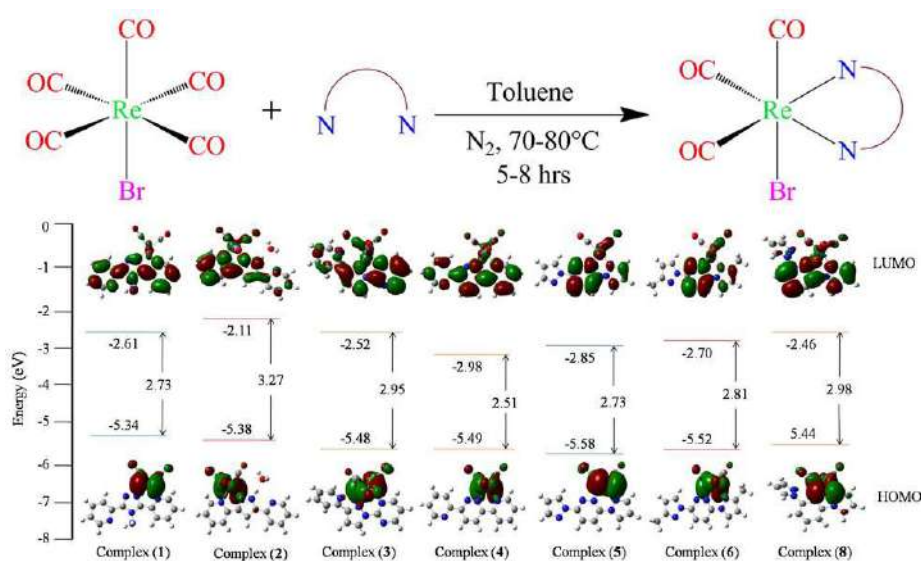
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Series of mononuclear rhenium(I) polypyridyl complexes have been synthesized by the reaction of $\text{Re}(\text{CO})_5\text{Br}$ with the corresponding N,N'-donor polypyridyl ligands (L1-L8) leads to the formation of mononuclear tricarbonylrhenium(I) complexes having the general formula *fac*- $[\text{Re}(\text{L})(\text{CO})_3\text{Br}]$ (**1-8**), where L = dpt-NH₂ (L1), Hbpp (L2), pypypm (L3), dpnp (L4), dpp (L5), dpp3Me (L6), dppMe (L7) and bpzpy (L8). All these nitrogen donor planar ligands react with the metal precursor under nitrogen atmosphere to form tricarbonylrhenium(I) complexes $[\text{Re}(\text{N}\cap\text{N})(\text{CO})_3\text{Br}]$ (**1-8**). All these metal complexes were isolated as neutral complexes and were characterized by FT-IR, ¹H NMR, UV-Vis and Mass spectroscopic techniques. These complexes (**1-6** & **8**) were structurally determined by single crystal X-ray diffraction technique. Single crystal X-ray crystallographic data conforms that the molecular structure of $[\text{Re}(\text{N}\cap\text{N})(\text{CO})_3\text{Br}]$ is distorted octahedron around the rhenium atom with one Br-atom, facial arrangement of three CO groups and one polypyridyl ligand. These mononuclear rhenium(I) polypyridyl complexes has the supramolecular structure with non-covalent interactions (hydrogen bonding, C-H... π and π - π [~ 3.421 Å] stacking). The molecular orbital diagrams of the complexes (**1-6** & **8**) have been obtained from the density functional theory (DFT) method. The spin-allowed singlet-singlet electronic transitions for the metal complexes $[\text{Re}(\text{N}\cap\text{N})(\text{CO})_3\text{Br}]$ have been calculated with the time-dependent DFT (TDDFT) method which are in good agreement with the experimental values.



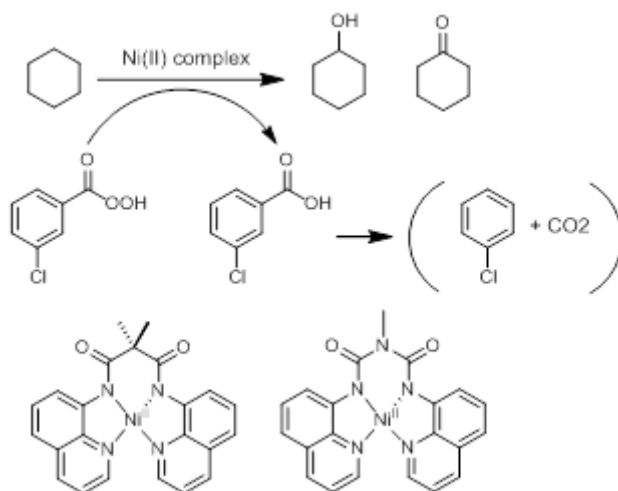
Ni(II) Complexes of Amido-Quinoline Liagnds as Catalyst for Alkane Hydroxylation Using *m*-CPBA

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Ni(II) complexes of a tetradentate-amido quinoline ligand was found to be a potent oxidation catalyst in catalyzing a series of alkanes having C-H bond dissociation energies ranging from 99.3 kcal mol⁻¹ (cyclohexane) to 84.5 kcal mol⁻¹ (cumene) using *m*-CPBA as an oxidant. We hypothesized that the reaction was going through the formation of Ni(III)-O[•] intermediate. ¹⁻³ EPR studies confirmed the formation of Ni(III) species in presence of *m*-CPBA.



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***In vitro* Investigation of Potential Anti-diabetic Activity of *Tribulus terrestris* L. by Modulating Hepatocyte Glucose Homeostasis**

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The epidemic of Type 2 diabetes mellitus necessitates development of novel therapeutic and preventative strategies to attenuate expansion of this debilitating disease. Type 2 diabetes mellitus is characterized by high blood sugar, insulin resistance, and defects in insulin secretion. Liver is the crucial organ which plays a central role in the maintenance of glucose homeostasis by balancing gluconeogenesis and glycogen synthesis. Over the past decades, several medications such as sulfonylureas, α -glucosidase inhibitors, biguanides, DPP-4 inhibitors are developed and used for the treatment of diabetes. However, most of these drugs are synthetic and are associated with adverse side effects, and resulted in poor prognosis and bioavailability along with other diabetic complications. Therefore, in recent times, traditional herbal medicines becoming popular and pharmacological evidences to understand the action of these medicines and underlying mechanisms to support the proper and safe use in clinic are indispensable.

The plant, *Tribulus terrestris* L., (*TT*) also known as Gokshura in Ayurveda, has a long history in the application for the treatment of diabetes and diabetic nephropathy. The plant also helps in lowering the level of serum glucose, serum triglyceride and serum cholesterol along with immunity boosting, aphrodisiac and rejuvenation properties. But pharmacological evidences to understand the action of the plant and underlying mechanisms is important. The study was aimed to investigate the therapeutic potential of the extract, fractions and isolated constituent(s) of *Tribulus terrestris* on hepatic insulin resistance in type 2 diabetes and to elucidate the underlying cellular mechanisms.

The seed of the plant *Tribulus terrestris* was extracted and fractionated using suitable solvents at normal room temperature. HPLC spectra was recorded for crude extract and different fractions. The crude extract along with its fractions are found to be effective in the uptake and utilization of glucose in *in vitro* conditions. All these results strengthen the hypothesis of using anti-diabetic potential of traditionally used *Tribulus terrestris* seeds. Therefore, further isolation of marker compounds from the active fractions and its characterization along with underlying mechanism of action must have to be carried out for the validation as antidiabetic agent.

Utilization of Fe(III)-impregnated HZSM5 as oxidation catalyst for removing industrial pollutants from water: A case study with 4-Nitrophenol

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Fe(III) impregnated ZSM5 as an effective catalyst for oxidation was prepared and used for the removal of aqueous 4-nitrophenol. Nitrophenols are toxic and persistent industrial pollutants and are included in the list of 130 priority pollutants by US EPA. The presence of the nitro group imparts enhanced acidic character that in turn affects the aquatic life in particular and the environment in general. Effluents containing these recalcitrant organics require tertiary treatment and catalytic wet oxidation has shown tremendous promise in this regard. In the present work, ZSM5 was first prepared by hydrothermal method and was transformed into HZSM and finally impregnated with Fe(III). The material was used as a catalyst for oxidation of 4-nitrophenol in water with or without the presence of oxidising agent H_2O_2 . The impregnated was done by refluxing hydrogen form of ZSM5 with aqueous 1M $Fe(NO_3)_3 \cdot 6H_2O$ for 6 hours. The structural features of the catalyst were determined with the help of powder XRD, SEM, TGA and FTIR measurements. The amount of Fe(III) entering onto the surface of HZSM5 was determined with the help of Atomic Absorption Spectroscopy(AAS).The material was calcined at 873K temperature before using as a catalyst. The oxidation was carried out in a high pressure stirred reactor at different time intervals and other process variables. As much as 94.55% conversion could be achieved. Results showed that with increasing time, catalyst load, mole ratio of H_2O_2 in the feed, the oxidative conversion could be further improved both in presence of the chemical oxidant and without it. Effects of various reaction conditions, kinetics of the catalytic process and the probable mechanism of oxidation have been discussed.

Key words: 4-Nitrophenol, Catalytic wet oxidation, Fe(III) impregnated HZSM5.

Study on Kinetics and mechanism of reaction between 2-Phenethyl alcohol and vinyl acetate catalysed by cross-linked *Pseudomonas Cepacia* lipase

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2-Phenethyl acetate (2-PEAc) is a highly valued ester with a rose-like odour that is widely used to add scent or flavor to cosmetics, soaps, foods and drinks. In this study, 2-PEAc was synthesized enzymatically by transesterification of vinyl acetate with 2-Phenethyl alcohol catalyzed by cross-linked enzyme crystals of *Pseudomonas Cepacia*. The solvent effect has been studied by using ten different solvents to correlate the initial rate with different solvent properties such as hydrophobicity, water solubility, electron pair acceptance and donation index, polarizability and dielectric constant. In this transesterification reaction, cyclohexane exhibits the highest initial rate. The effect of synthesis parameters on the conversion of 2-PEAc was evaluated. The reaction follows Ping-Pong-Bi-Bi mechanism with substrate inhibition.

Keywords: Transesterification, solvent effect, cyclohexane, Ping-Pong-Bi-Bi

Tuning of Halogen-Bond Strength: Comparative Role of Basicity and Strength of σ -Hole

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The halogen bond is highly directional and tunable in nature. Directionality is explained by the anisotropy in electron distribution around the halogen atom in a molecule, which eventually increases its electrostatic attraction at the preferred direction with any electronegative molecular entity. The electron deficient region is popularly known as σ -hole [1]. A theoretical study has been carried out on the N...Cl halogen bonded complexes between various halomethanes and ammonia derivatives at the MP2=Full/aug-cc-pVTZ level of theory. The binding strength of these complexes ranging between -2.04 and -13.55 kJ/mol are found to correlate well with parameters like positive electrostatic potential (V_{\max}) on the Cl atom and the proton affinity (PA) of the N-bases. Further, the dominant role of V_{\max} on Cl atom over the proton affinity of N-bases in stabilizing the halogen bonded complexes has been discussed in detail. SAPT [2] analysis reveals the important role of σ -hole in determining the electrostatic interaction energy. The role of $\rho(r_c)$ at the BCP in stabilizing the halogen bonded complexes has also been discussed employing AIM [3] analysis.

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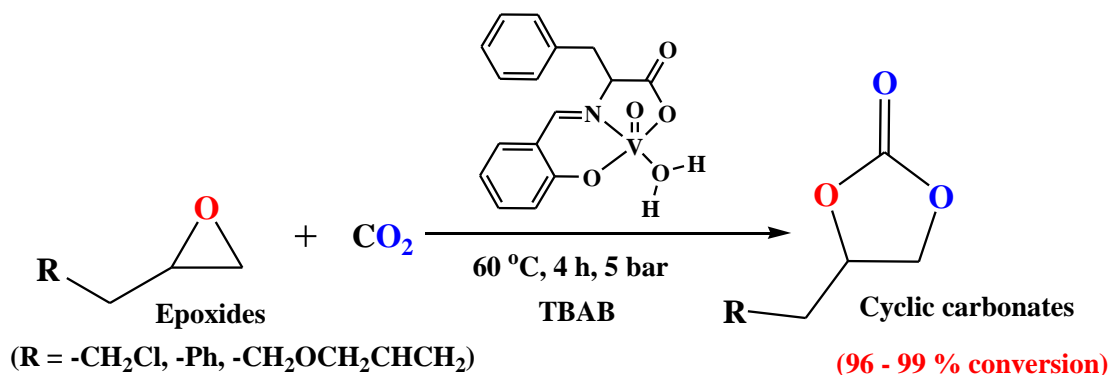
Synthesis of Cyclic Carbonates from Epoxides and CO₂ catalysed by a (L)-phenylalanine derived Schiff base ligated Vanadium(IV) complex

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The chemical fixation of CO₂ via a cycloaddition reaction with epoxides for synthesizing valuable cyclic carbonates is a widely studied atom economical reaction. The cyclic organic carbonates have wide applications as protic solvents, electrolytes in Li batteries, and as raw materials for many polymerization reactions. In this work, an oxovanadium(IV) complex, V^{IV}O(sal-L-phe)(H₂O), involving an (L)-phenylalanine based Schiff base ligand has been synthesized by a one pot reaction between salicylaldehyde, (L)-phenylalanine and vanadyl sulphate at room temperature, and characterized by IR, UV-Vis and ESI-MS spectrometry. The vanadium (IV) complex, when kept for crystallization in methanol, undergoes oxidation to give the crystals of a vanadium (V) complex, V^VO(sal-L-phe)(OCH₃)(HOCH₃). The crystal structure analysis has revealed the formation of the vanadium (V) complex, with a methoxide ligand and a neutral methanol ligand coordinated to the vanadium centre, from the parent vanadium (IV) complex. The parent vanadium (IV) complex, V^{IV}O(sal-L-phe)(H₂O), has been used to study the synthesis of cyclic carbonates via the cycloaddition reaction of epoxides and CO₂ and has proved to show efficient catalytic activity under mild reaction conditions. Conversions of 96-99% has been achieved at 60 °C temperature and 5 bar pressure of CO₂ after only 4 hr using the vanadium (IV) complex, V^{IV}O(sal-L-phe)(H₂O).



Detection of DNA lesion and current effort toward targeting cancer cell DNA

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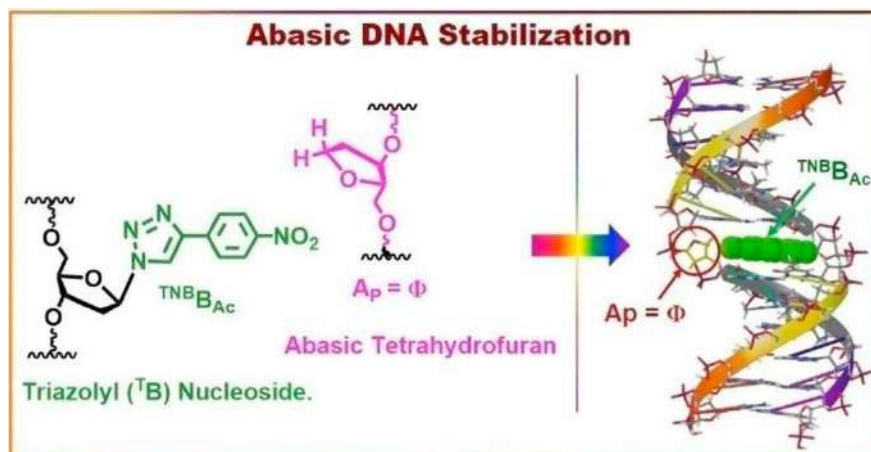
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In the field of genomics DNA, apart from oxidative cleavage and single strand break, formation of abasic site is one of the most common observed phenomenon. It takes place due to cleavage of the glycosidic bond, an exogenous agent or failure of base excision repair machinery (BER). Under physiological condition these abasic sites are formed spontaneously due to depurination and their formation can cause misincorporation of the nucleotide triphosphate during DNA replication by the Polymerase enzyme. Thus, formation of abasic site is one of the reasons for chemically induced mutation and cell death.

Base Excision Repair Mechanism plays an important role by efficiently repairing the abasic site thereby preventing further damage. However, if unrepaired due to failure of BER mechanism this might lead to single nucleotide polymorphism, block transcription, stop DNA replication. Thus the need of the hour is to find ways to measure extent of DNA damage, methods of identification and stabilization of these abasic sites. Stabilization and identification of these abasic sites can lead to development of new diagnostics and chemotherapeutics.

Our work is directed toward the stabilization of these abasic sites via pairing them with bulky triazole based unnatural nucleoside. These modified nucleoside must be of similar characteristics and volume so as to fit well into the cavity by intercalative mechanism.



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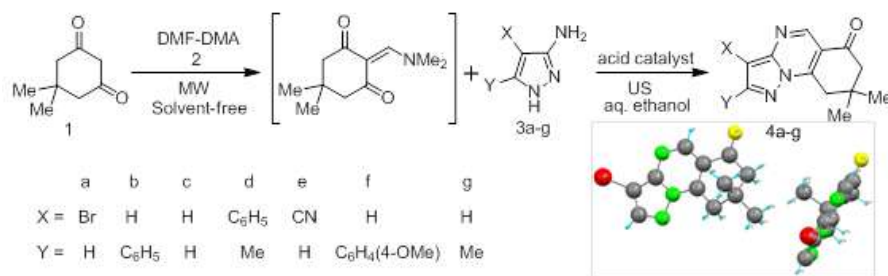
A simple, facile and green synthetic protocol to obtain various Pyrazolo[1,5-*a*]quinazoline derivatives

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Pyrazolo[1,5-*a*]quinazoline derivatives, tricyclic molecular systems, have wide range of applications in the field of medicine such as anti-bacterial [¹], anti-cancer [²], anti-oxidant [³], anti-inflammatory [⁴], anti-diabetic [⁵], anti-viral [⁶] and pesticides [⁷] owing to their unique structure. These have fuelled various studies in search of novel synthetic route to harvest this important heterocyclic entity. According to the literature reports [5, 8], the synthetic procedures utilized to acquire these molecules are harmful to the environment. Thus, in continuation with our modest contributions [⁹] on the synthesis of biologically important heterocyclic molecules we present herein a straightforward, rapid, effective, high yielding and environmentally friendly synthetic methodology for the synthesis of these molecules. Our method involves mild catalyst, US irradiation and aq. solvent with high atom economy. The structures of the products were confirmed with the help of their spectral data (¹HNMR, ¹³CNMR, FT-IR and Mass Spectrometry). For further confirmation of their structures, a compound was selected as model compound and its single-crystal X-ray crystallography analysis was done and is presented herein.



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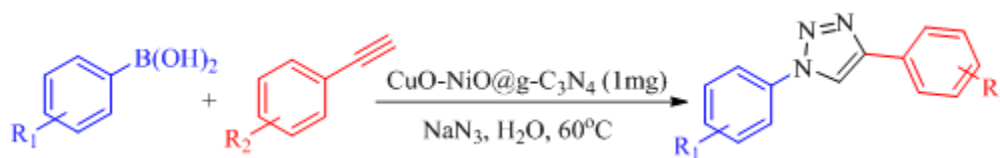
Synthesis of biologically active triazoles catalyzed by graphitic carbon nitride supported bimetallic CuO-NiO.

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A highly efficient and reusable graphitic carbon nitride supported bimetallic CuO-NiO catalyst has been developed. The incorporation of CuO-NiO on the surface of graphitic carbon nitride has been confirmed by several spectroscopic techniques such as FT-IR, SEM, TEM-EDX, SAED, PXRD, RAMAN, TGA and XPS. After the successful characterization of the catalyst, it was successively employed for the synthesis of biologically and industrially active triazoles¹⁻² from phenyl boronic acids, sodium azide and phenyl acetylenes in aqueous medium. The process emerged to be very efficient providing several benefits such as short reaction time, good yields, use of environmentally benign solvent and reusability of the catalyst.



Scheme 1: Synthetic scheme for triazoles.

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Removal of dye from Aqueous Solution Using Bio-adsorbents.

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Contamination of surface and groundwater with industrial effluents is becoming a major threat to human health as well as aquatic life. Among the various hazardous materials that contaminate water, dyes released from textile, photographic and dyestuff industries, and heavy metals released either naturally through a variety of geochemical processes or by direct discharge of municipal and industrial wastes, are of particular environmental concern. There has been increasing scientific concern about the hazardous effects of colored dyes.

The main objective of this present study to investigate the feasibility of Bioadsorbent Bokul (*Mimusops eleng*) leaf powder (BLP), Bokul leaf ash (BLA) and Banana pseudo-stem ash (BSA) as an efficient adsorbent for the removal of methylene blue dye and Pb(II) from water. The present study is carried out with respect to Characterization of Bioadsorbents, Batch studies in terms of pH, Agitation, Concentration, Time, Isotherm Model and Kinetic Studies.

In this present investigation the predominant findings are, pH of bokul leaf powder, bokul leaf ash and banana pseudo stem ash are found to be 5.6, 9.6 and 10.0 respectively. The surface areas of BLP, BLA & BSA are found to be 26.2 m²/g, 45.4 m²/g, and 227.8 m²/g respectively. The bulk densities of BLP, BLA & BSA are found to be 0.24 g/cm³, 0.41 g/cm³ and 0.23 g/cm³ respectively. In the batch studies it has been observed that pH has significant influence on adsorption. It is observed that the optimum pH for Methylene Blue removal is 4, 12, 2 for BLP, BLA, BSA respectively, and optimum pH for Pb(II) removal is 2, 8, 10 for BLP, BLA, BSA respectively. The equilibrium time obtained for adsorption of Methylene Blue onto BLP, BLA, and BSA adsorbents are 90, 90, 120 min respectively and the equilibrium time for the adsorption of Pb(II) onto BLP, BLA, BSA adsorbents are 60, 75, 75 min respectively. The adsorption of both Methylene Blue and Pb(II) onto Bokul leaf powder, Bokul leaf ash and Banana pseudo-stem ash follows second order kinetics.

In this present Study it can be concluded that the Methylene Blue and Pb(II) are efficiently removed from the aqueous solutions by adsorption process using Bokul leaf powder, Bokul leaf ash, and banana pseudo-stem ash.

Antioxidant properties of Folic acid Analogue anti-cancer drugs: A DFT study

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Antioxidant properties of 4 folic acid analogue anti-cancer drug molecules namely methotrexate, aminopterin, talotrexate, trimetexate have been investigated using density functional theory (DFT)-based computational methods. The O–H bond dissociation energy (BDE), proton dissociation energy (PDE), proton affinity (PA), electron transfer energy (ETE) and ionization energy (IE) were calculated in the gas phase at the ROB3LYP/6-311++G(2df,2p)//B3LYP/6-311G(d,p) level of theory. Quantum chemical descriptors namely chemical potential (μ), chemical hardness (η), global electrophilicity (ω) were calculated in order to evaluate the reactivity and stability of all studied compounds. The main conclusion drawn from the investigation is that hydrogen atom transfer (HAT) and single electron transfer (SET) are the main mechanism of antioxidant behaviour of these compounds.

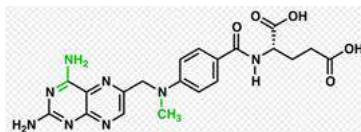


Figure : Structure of methotrexate

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Electrocatalytic water oxidation by Cu (II) complexes in aqueous Medium

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Electrocatalytic oxidation of water by transition metal complexes is a highly active field of research at the present time due to its implications in the conversion of electrical energy into chemical fuel.¹⁻³ A large number of metal complexes have been reported with the ability of electrocatalytic oxidation of water in neutral, acidic and basic media. In view of cost effectiveness and robustness, copper based complexes have emerged as potential water oxidation catalysts. Since the report of the first copper based electrocatalyst by Mayer et al.,¹ a large number of copper complexes have been reported with successive improvements in catalytic activity.⁴⁻⁶ In the present work, we have described the synthesis and electrocatalytic activity of a copper (II) complex, with Histidine based ligand. Electrochemical studies of the copper (II) complex depict that it behaves as a potent water oxidation catalyst exhibiting high catalytic efficiency.



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Phytoplankton community structure and abundance in an aquaculture pond of Guwahati, Assam

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With the standpoint of the role of phytoplankters as primary producers in aquatic ecosystems, the present investigation was undertaken in an aquaculture tank to study the phytoplankton community structure and abundance for a period of one year from the month of January to December in 2016. Phytoplankton samples were collected from the sub-surface water with the help of a nylobolt plankton net (No. 25) for both qualitative and quantitative analysis. Identification of phytoplankton species is done up to genus level while the abundance is expressed in unit cell per litre (ul^{-1}). Surface water samples were collected to study the physico-chemical parameters – temperature, pH, dissolved oxygen (DO), free carbon dioxide (FCO), total alkalinity (TA), total hardness (TH), chloride (Cl^-), Calcium (Ca^{2+}), Magnesium (Mg^{2+}) and transparency. Multivariate correlation was determined among the phytoplankton groups and the abiotic parameters to find out their interrelationships.

A total of 43 phytoplankton genera belonging to 19 families under 6 classes namely Myxophyceae, Chlorophyceae, Euglenineae, Dinophyceae, Chrysophyceae and Bacillariophyceae were recorded in the sampled pond. The group Chlorophyceae registered the highest richness with 20 genera followed by the groups Bacillariophyceae (9 genera), Myxophyceae (7 genera), Dinophyceae and Euglenineae each with 3 genera and Chrysophyceae with a single genus. The phytoplankton abundance ranged from 484- 10919 \pm 2862 ul^{-1} . The group Chlorophyceae hold the highest rank (69.5%) in the percentage contribution to the phytoplankton abundance while the lowest was the group Bacillariophyceae (1.9%). The trend of phytoplankton abundance different seasons can be represented as - monsoon (June to August) > pre monsoon (Mar to May) > retreated monsoon (Sept to Nov) > winter (Dec to Feb).

Diversity indices estimated among the phytoplanktonic groups revealed the highest value for Shannon_H (1.37), Simpson index (0.59) and Margalef (1.73) indices in the group Chlorophyceae while maximum Evenness is found in the group Bacillariophyceae.

The multivariate correlation analysis revealed a negative and significant ($p < 0.05$) correlation between – Myxophyceae and TA, Myxophyceae and pH, Chlorophyceae and Transparency, Euglenineae and Cl^- ; whereas significant ($p < 0.05$) positive correlation was recorded between – Myxophyceae and TH, Myxophyceae and pH, Chlorophyceae and Chloride, Dinophyceae and TA, Bacillariophyceae and DO.

Key words: Aquaculture pond, abundance, diversity, phytoplankton

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