Recent Trends in Chemical Sciences - 2022

RTCS
2022

December 16-18, 2022

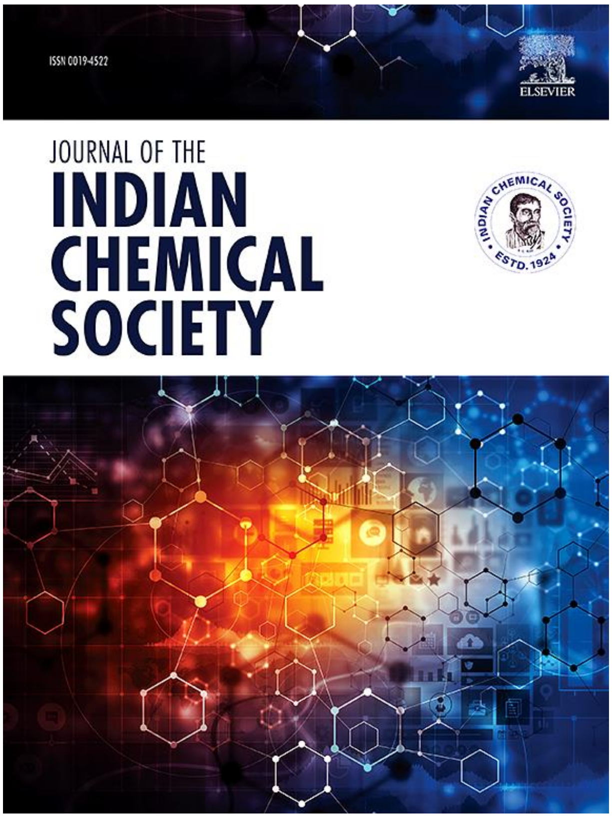
Abstracts

Organized by

Department of Chemistry & Chemical Biology
Indian Institute of Technology (ISM) Dhanbad, India

About Indian Chemical Society

The Indian Chemical Society, a premier Scientific Society of India, was founded in 1924, as National Forum for the community of chemists and members of allied disciplines in the country. The driving force behind its establishment was the nationalistic spirit prevailing in India under British rule. J. N. Mukherjee, J.C. Ghosh and S.S. Bhatnagar while carrying out their research work in the University College, London in 1919 for the D.Sc. Degree, took a decision that after coming back to India their endeavor would be to establish a Chemical Society like the Chemical Society of London. Their cherished dream was transformed into a reality with active cooperation of many of the leading personalities in the country, and the Indian Chemical Society was founded on May 9, 1924, as a registered Society, with Sir Prafulla Chandra Ray, the doyen of Indian Chemists, as the first President. Many of the distinguished personalities in the field of Chemical Science of that time in India took active interest in nurturing the new born Society.



About IIT (ISM) Dhanbad

The Indian National Congress at its XVII Session of December 1901 passed a resolution stating that "in view of the fact that the tendency of recent legislation namely, The Indian Mines Act VII of 1901, is that all Indian mines must be kept under the supervision of mining experts, the Congress is of opinion that a Government College of Mining Engineering be established in some suitable place in India on the models of the Royal School of Mines in England, Mining Colleges of Japan and at other places in the continent". The McPherson Committee formed by Govt. of India, recommended the establishment of an institution for imparting education in the fields of Mining and Geology, whose report, submitted in 1920, formed the main basis for establishment of the Indian School of Mines, Dhanbad.

The Indian School of Mines was formally opened on 9th December 1926, by Lord Irwin, the then Viceroy of India to address the need for trained manpower related to mining activities in the country with disciplines of Mining and Applied Geology. In 1967 it was granted the status of a deemed to be university under Section 3 of UGC Act, 1956. Since its establishment, IIT(ISM) has undergone considerable expansion of its activities, and presently it can be considered as a total technology education institute.

Director's Message

I am delighted that the Department of Chemistry and Chemical Biology, IIT(ISM), Dhanbad is hosting a three-day international conference on "**Recent Trends in Chemical Sciences-2022 (RTCS-2022)**" in the campus from 16th to 18th December 2022.

Chemistry is ubiquitous in daily life. Globally, the pace of chemical research is transforming into multidisciplinary areas, focusing on human wellbeing. This progress of the translation is leaping forward day-by-day with the advancement of research on different areas, like novel materials, chemical biology and affordable synthesis. The Department of Chemistry and Chemical Biology, IIT(ISM) Dhanbad is dynamic with a vast reserve of brilliant faculties, who provide new avenues for students towards exciting prospects of research. There is a critical need for R&D in various disciplines of Chemistry and the list is unending. This is only possible with the constant exchange of ideas and knowledge, which is one of the main mottos behind organizing conferences and seminars, like the current one.

I extend my best wishes for the conference RTCS-2022, and am confident that this meeting will be a great success and benefit to all the participants.

Prof. Rajiv Shekhar
Director
IIT (ISM), Dhanbad

INDIAN CHEMICAL SOCIETY

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Professor G.D. Yadav
President

Professor Chittaranjan Sinha
Honorary Secretary

To

All the Fellows of the Indian Chemical Society
and Fellow Chemists of all Academic Institutes

Dear Friends and Colleagues,

The Indian Chemical Society, a premier Scientific Society of India, was founded in 1924, as National Forum for the community of chemists and members of allied disciplines in the country. The driving force behind its establishment was the nationalistic spirit prevailing in India under British rule. J. N. Mukherjee, J.C. Ghosh and S.S. Bhatnagar while carrying out their research work in the University College, London in 1919 for the D.Sc. Degree, took a decision that after coming back to India their endeavour would be to establish a Chemical Society like the Chemical Society of London. Their cherished dream was transformed into a reality with active cooperation of many of the leading personalities in the country, and the Indian Chemical Society was founded on May 9, 1924, as a registered Society, with Sir Prafulla Chandra Ray, the doyen of Indian Chemists, as the first President. Many of the distinguished personalities in the field of Chemical Science of that time in India took active interest in nurturing the new born Society.

The Indian Chemical Society is presently involved in various academic activities which have drawn attention of the Chemists of other countries. Its future depends on sincere, honest and vigorous efforts of its Fellows and Members. Annual Convention of Chemists is a yearly event of the Society and last two years whole world has suffered much of Covid-19 and like other countries we remained lockdown. Our scientific activities and administrative works were performed from ‘home’. The Society organised academic activities through on-line. The Journal of the Indian Chemical Society is being published from 2021 by the Elsevier Publishing House and has received tremendous response with submission of over 3000 articles so far. About 70% articles were rejected due to strict criteria of plagiarism and refereeing standards. The Journal is ahead of its publication schedule and already 2023 articles are online.

The physical program is resumed and the 59th Annual Convention of Chemists 2022 is being organized on December 16–18, 2022 at the Department of Chemistry and Chemical Biology, Indian Institute of Technology (ISM) Dhanbad, Jharkhand. The programme of the consists of Scientific Sessions in Seven different Sections. Seven different Sections are (i) Physical Chemistry, (ii) Organic & Biochemistry, (iii) Inorganic Chemistry, (iv)Analytical Chemistry, (v) Environmental Chemistry, (vi) Industrial & Applied Chemistry, (vii) Chemical Engineering & Green Technology.

The Society intends particularly to encourage the budding young chemists of our country by organizing special award sessions to accommodate the contributions of the young chemists. It gives me immense pleasure to announce new Awards as will be selected by the Juries team in addition to Annual Convention Awards to young Chemists (age ≤ 35 y). Lifetime Achievement Awardees, Endowment Awardees, Senior Scientists of the country and abroad will join along with Young Scientists of the country in this Convention. ACS, RSC and Elsevier have agreed to sponsor some awards.

I believe that the Convention would provide an effective platform for exchange of thoughts among the participating chemists which would be able to generate new ideas and open up new fields of research.

I earnestly hope that chemists from our country and abroad will participate in this Convention to make it a grand success.

The Society will go into its centennial year in 2023 with many activities across the country. I am sure you will be part of the grand celebration.

With regards,

Yours sincerely,

GD Yadav

G.D. Yadav
President
Indian Chemical Society

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Professor G.D. Yadav
President

Professor Chittaranjan Sinha
Honorary Secretary

Message from Honorary Secretary
Dear Fellows, Members & Participants,
Greetings from Indian Chemical Society!

The years 2020 and 2021 were went off with COVID-19 Psychosis along with growth of all-round digital technology. Indian Chemical Society exploited this technology throughout last couple of years by organising students' competition, Research Scholars program, national and international conferences, symposia, seminars and workshops. The off-line Annual meeting was held last in 2019 in Pt. Ravisankar Shukla University and is going to held again in this year in IIT(ISM), Dhanbad. The Society has bestowed Lifetime Achievement Awards to very senior scientists, Endowment Awards to senior scientists and 'Young Scientist Awards' in the Annual Convention. Every year the Society is organising Students' program to celebrate National Science Day, Foundation Day Celebration (9th May), August Symposium to commemorate Birthday of Acharya Ray (2nd August) and Annual Convention of Chemists. Besides, many collaborative programs with Colleges, Universities and research institutes are organised religiously. The *Azadi Ka* Amrit Mahotsav is celebrated on August, 2022 as a part of 75th Year of Indian independence in hybrid mode: International Research Scholars competition was organised virtually and August Symposium by off-line mode. In addition to the conferences, the Society publishes Books, Periodicals and a journal of international standard. The newsletter, Chem Warta, is regularly uploaded in the Website of the Society (www.indianchemicalsociety.com). The Journal of the Indian Chemical Society is published (2021) by the Elsevier. All the issues of the journals are now freely available (1924-2020) in the Society Website. For young scientists the Society initiated S. S. S. Bhatnagar Young Chemist Award and Indian Chemical Society Research Excellence Award in addition to Young Scientist Awards (age □ 35 y) contributed by the different persons. The Society is waiting for ISSN to publish a new quarterly journal "Accounts of Chemical Education and Research (ACER)".

Members and Fellows are the power of the Society. Life Fellows, Life Members, Institute Members, Corporate Members and Student Members govern the Society. More than 3000 members/fellows of the Society are associated with five zones (Head Quarter, East, west, North and South) along with few branches like Allahabad, Bhagalpur, Chennai, Mumbai, Raipur, Vadodara, Jalandhar, North-East in the country. Both the Branch and Zone have independency to popularise the Society through different scientific activities with information to the Office. Our enthusiastic high esteemed visionary President, Prof. G. D. Yadav is instrumental to all the activities and has committed to collect funds and human resources to restore the glorious past of the Society. It feels to share with you that the Society is being approached by the scientists, researchers and scientific organisations nationally and internationally with different specialties for collaborative program. One of the disappointing news is that the Society has not yet started to build '**Acharya Bhawan**' on their own land due to some non-technical issues. Our yearly programs are well received and we find that the number of participations is increasing every year. The statue of Acharya Ray is unveiled in the Head Office of the Society during the August program in this year.

The Society conveys heartfelt thanks and gratitude to the members of the Local Organising Committee, International Advisory Committee and the Head & the members of the

Department of Chemistry and Chemical Biology and the highly enthusiastic research scholars in particular and the Director, The Dean & Staff, Indian Institute of Technology (ISM), Dhanbad in general for their all-out efforts and to make this program successful at very short time gap. Our great salute to your earnest support, selfless striving and in-depth emotion towards growth of nationalistic spirit through the service to the chemistry and to materialise the dream of Acharya Ray for improving the Society’s health and activity.

Thanks to all Lifetime Achievement Awardees, Endowment Awardees, Fellows, Members, Advisors, Patrons and the Members of the Council for timely suggestion, continued support and guidance. Last but not the least is our only few employees in the Head Quarter in Kolkata who bear this heavy responsibility silently with inadequate financial support.

I do hope that you will enjoy the three days program, interact with experts, exchange your ideas and dreams and will improve the all-round growth of the Society. In spite of the best efforts some involuntary errors might have crept in for which I tender my sincere apology.

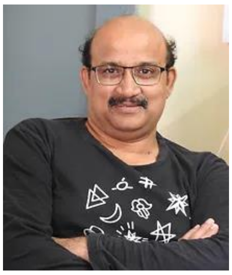
Best wishes all for a successful conference. Looking forward to the next year!

Chittaranjan Sinha

(Chittaranjan Sinha)
Honorary Secretary
Indian Chemical Society

13th December, 2022

HoD’s Message



Welcome to the International Conference on Recent Trends in Chemical Sciences- 2022 hosted by the Department of Chemistry and Chemical Biology, Indian Institute of Technology (Indian School of Mines), Dhanbad. On behalf of the faculty, staff and students of our department, I invite you to this conference and explore the vibrant activities in our department. While our expertise in research includes the traditional areas of physical, inorganic, organic and analytical chemistry, we are rapidly expanding the horizon to interdisciplinary fields of chemical biology, drug discovery, materials chemistry, theoretical chemistry and nanotechnology. The department is well-equipped by state-of-art instrumentation facilities in the research and UG-PG labs, and is also supported by the central research facility of the institute. In addition to the Ph. D. program, the department offers two Masters programs (M.Sc. Chemistry and M. Tech in Pharmaceutical Science and Engineering), wherein, students get the opportunity to work with the faculty members in their ongoing research or opt for an industry internship. We strive to conduct relevant research and to provide learning opportunities to students to get trained as next-generation scientists.

Your suggestions to promote the Department to greater heights are most welcome.

Best wishes!

Prof. Parthasarathi Das
Head of Department
Chemistry and Chemical Biology

Message from
Convenor
Local Organizing Committee
RTCS-2022

It is with great pleasure, I welcome you all to the "**Recent Trends in Chemical Sciences-2022** (**RTCS-2022**)" organized by the Dept. of Chemistry and Chemical Biology, IIT(ISM) Dhanbad under the aegis of Indian Chemical Society, Kolkata from 16th to 18th December, 2022. This conference is intended to provide a valuable forum for various branches of chemical science and chemical engineering in India and beyond to come together at a common place and facilitate exchange of ideas. The mission of this programme is to provide a wonderful platform annually for researchers from India and around the globe to present their technical findings in different fields of chemistry related research that can lead to networking and broader multi-disciplinary research collaborations.

With the hope that everyone takes some valuable insights back from these three days, I wish all the participants and delegates a very effective 3 days event at Indian Institute of Technology (ISM) Dhanbad. I am sure that this RTCS -2022 would be a wonderful experience for everyone present here.

Sagar

Sagar Pal
Convenor, Local Organizing Committee
RTCS-2022

Message from
Co-Convenor
Local Organizing Committee
RTCS-2022

It is with immense pleasure that I welcome you all to **"Recent Trends in Chemical Sciences – 2022"** being hosted by Indian Institute of Technology (ISM) Dhanbad, under the aegis of Indian Chemical Society. I am proud to be part of this confluence of the rich heritages of IIT (ISM) and the Indian Chemical Society - the oldest Chemical Society of India that is being borne out by this event. As part of the team of organizers, we have tried to bring together some of the brightest minds that are engaged in cutting edge research in the frontier areas of the Chemical Sciences and allied fields. Encompassing seven parallel technical sessions, spread out over three days, we hope to achieve a wide dissemination of the new and exciting research of the speakers through a series of Endowment Lectures, Invited Lectures and Oral Presentations. I also believe that the poster sessions will help to engage young researchers to present their recent work through engagement with the more experienced chemists as well as among themselves. In addition to the technical sessions, we hope the delegates and participants enjoy the cultural program in the evenings.

I thank you all for participating in this conference and starting off its journey towards a hugely successful event. Finally, I hope that all of you enjoy your stay here at IIT (ISM) Dhanbad, partaking in a hearty exchange of scientific ideas while being briefly acquainted with the local culture and cuisine of the state of Jharkhand.

Best wishes!

Somnath Yadav

Somnath Yadav
Co-Convenor, RTCS-2022

Chief Guest's Message

It gives me immense pleasure to note that Department of Chemistry and Chemical Biology, Indian Institute of Technology (ISM) Dhanbad is hosting the 59th Annual Convention of Chemists under the aegis of Indian Chemical Society, the oldest professional body in India which is engaged in promoting Chemical Sciences, Engineering and Technology for the last 99 years with the initiative of Prafulla Chandra Ray, the father of Modern Indian Chemistry as First President.

I congratulate IIT (ISM) Dhanbad for hosting such an important conference on the theme *"Recent Trends in Chemical Sciences"* that would deliberate on the recent trends in chemical sciences and hope the discussions will focus on the multiple sub-disciplines of chemistry and will provide the platform for the scientists, researchers, and students to learn and accelerate vistas of growth in the latest advancements in the field of chemical sciences. This platform will bring together the brightest minds from various sectors of the industry and it will be an ideal place for exchanging ideas. Let us all learn from these ideas and take the world forward by working out on developing highly selective, energy efficient and environmentally benign new synthetic methods and processes that are greener by design. This is desired to help meet the challenges of preserving the environment, developing renewable energy sources, discovering drugs, and synthesizing nanoscale materials and making changes in the existing environment to deliver better products and services.

I extend my heartiest wishes to the Conference Organizers and all associated persons who have been working with their complete dedication and efforts to make this International Conference on Recent Trends in Chemical Sciences -2022 (RTCS-2022) a reality. Eventually I express my special thanks and appreciation to all and wish that the IRTCS -2022 becomes a grand success and a benchmark for all forthcoming conferences in India and abroad.

Regards

Vibhash Kumar
Executive Director & State Head, Bihar and Jharkhand
Indian Oil Corporation Ltd

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Professor G.D. Yadav
President

Professor Chittaranjan Sinha
Honorary Secretary

LIFETIME ACHIEVEMENT AWARD, 2022

CONFERRED ON

Professor Kankan Bhattacharyya, FNA

Members of the Council and the Fellows of the Indian Chemical Society feel honoured to felicitate Professor Kankan Bhattacharyya in recognition of his lifetime achievement in research in the field of Chemistry in general and Physical Chemistry in particular.

Professor Kankan Bhattacharyya was an eminent physical chemist of international acclaim. Almost all of his research career was in the Indian Association for the Cultivation of Science, Kolkata. After his retirement, he was appointed a Visiting Professor at IISER Bhopal. His pioneering work on the low dynamics of biological water generated a lot of excitement world-wide and kickstarted a flurry of activity. Starting with picosecond spectroscopy, Professor Bhattacharyya went on to investigate Femtosecond dynamics of photoprocesses in complex environments. He made important advances in understanding processes like excited state electron and proton transfer, photoisomerization, FRET etc. At a rather advanced stage in his career, he ventured into time resolved fluorescence microscopy in soft matter and live cells. In doing so, he developed a unique physical chemist's perspective of these systems.

In recognition of his scholastic activities, Professor Bhattacharyya received many awards and accolades. To name a few, he received the Shanti Swarup Bhatnagar prize and was a Fellow of all the three Indian Academies of Science. He received TWAS prize and was admitted to the fellowship of TWAS.

Professor Bhattacharyya served as the Director, Indian Association for the Cultivation of Science and was a Senior Editor of the Journal of Physical Chemistry for a long time. His eminence was recognised this year, through the publication of a Virtual Special Issue: Kankan Bhattacharyya Festschrift.

A dedicated academician, Professor Bhattacharyya had contributed significantly to the development of Chemical research in the Country and also inspired a large number of students and colleagues who are now carrying the torch of his mission.

GDYadav

Professor G.D. Yadav
President
Indian Chemical Society

Chittaranjan Sinha

Professor Chittaranjan Sinha
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Professor G.D. Yadav
President

Professor Chittaranjan Sinha
Honorary Secretary

LIFETIME ACHIEVEMENT AWARD, 2022

CONFERRED ON

Professor Sisir Chandra Rakshit

Members of the Council and the Fellows of the Indian Chemical Society feel honoured to felicitate Professor Sisir Chandra Rakshit in recognition of his Lifetime Achievement in teaching and research in the field of Chemistry in general and Theoretical Chemistry in particular.

Professor Rakshit joined as Professor in the Department of Chemistry, The University of Burdwan and rendered his dedicated service for more than three decades. He was an illustrious teacher and had taught mainly Physical Chemistry based courses such as Quantum Mechanics, Spectroscopy, and Group Theory.

Research work of Professor Rakshit covered both theoretical and computational aspects of the Physical Chemistry. He had authored several numbers of text book including "Atomic and Molecular Symmetry Groups and Chemistry", "Atoms and Dn Ions in Perturbation Fields" and "Symmetry Theory: Principles, Molecules and Atoms: Problems and Solutions for Chemists".

Professor Rakshit greatly inspired and influenced his students to choose this fascinating field of research by his motivational teaching. Apart from it, many of his students are world leaders to in various academic institutions.

A dedicated academician, Professor Rakshit has contributed significantly to the development of Physical Chemistry in the Country and also inspired a large number of students and colleagues who are now carrying the torch of his mission.

The Indian Chemical Society sincerely wishes Professor Rakshit a long peaceful life with sound health and continuous academic activities for the advancement and propagation of Scientific Knowledge.

GDYadav

Professor G.D. Yadav
President
Indian Chemical Society

Chittaranjan Sinha

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Professor G.D. Yadav
President

Professor Chittaranjan Sinha
Honorary Secretary

LIFETIME ACHIEVEMENT AWARD, 2022

CONFERRED ON

Professor Narayanasami Sathyamurthy, FNA

Members of the Council and the Fellows of the Indian Chemical Society feel honoured to felicitate Professor Narayanasami Sathyamurthy in recognition of his lifetime achievement in teaching and research in the field of Chemistry in general and Physical Chemistry in particular.

Professor Sathyamurthy was the founder Director of prestigious Indian Institute of Science Education and Research, Mohali, in the year 2007 and continued his dedicated service till 2017 as the Honorary Professor. He was elected the President of Chemical Research Society of India from 2017-2020. He had served as the former Institute Chair Professor at the Indian Institute of Technology, Kanpur. For his outstanding research contributions in the field of molecular research dynamics, non-adiabatic interactions, atomic and molecular clusters in free state as well as under confined conditions and more than two-hundred research publications, he had received worldwide attention and appreciation from the academic field and achieved several awards and distinctions for his academic contribution. To mention a few are the S.S. Bhatnagar Award in Chemical Sciences, and Rev. Yedanapalli Memorial Award from the Indian Chemical Society.

In recognition of his scholastic activities, Professor Sathyamurthy had been elected Fellow of the Indian Academy of Sciences, Bengaluru and Indian National Science Academy, New Delhi and The World Academy of Sciences, Trieste, Italy.

Professor Sathyamurthy being an Editor and Member of different Editorial Board of different Journals, had edited a book of entitled “Reaction Dynamics: Recent Advances”. He was also the Chief Editor, Editor, and Member of several Editorial Boards of those Journals, like Resonance-Journal of Science Education, published by Indian Academy of Sciences, Bengaluru.

A dedicated academician, Professor Sathyamurthy has contributed significantly to the development of Chemical research in the Country and also inspired a large number of students and colleagues who are now carrying the torch of his mission.

The Indian Chemical Society sincerely wishes Professor Sathyamurthy a long peaceful life with sound health and continuous academic activities for the advancement and propagation of Scientific Knowledge.

Chittaranjan Sinha

Professor G.D. Yadav
President
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LIFETIME ACHIEVEMENT AWARD, 2022

CONFERRED ON

Professor S.T. Nandibewoor

Members of the Council and the Fellows of the Indian Chemical Society feel honoured to felicitate Professor S.T. Nandibewoor in recognition of his lifetime achievement in teaching and research in the field of Chemistry in general and Physical Chemistry in particular.

Professor S.T. Nandibewoor had published more than five hundred scientific papers in National and International peer reviewed Journals. His works were much appreciated and indexed and cited in various peer reviewed journals, scientific reviews and text books and had achieved more than 7500 citations with 42 h-index. He has successfully guided 50 Ph. D students and 6 M. Phil students. Thirty five students of Professor Nandibewoor have received Young Scientist Awards. He has already completed twelve research projects and currently guiding three Ph.D students. He used to travel different foreign countries on different academic assignments to different Universities.

Professor S.T. Nandibewoor had received worldwide attention and appreciation from the academic field and achieved several awards and distinctions for his academic contribution. To mention a few, Professor Nandibewoor was the recipient of "Educationist Medal" by Akhila Bharat Veershavia Samaj, 2002, "Best Research Publication Award 2010" by Government of Karnataka, Bangalore, "Professor Malik Memorial Award 2011" by Indian Council of Chemists, Agra, "Certificate of Appreciation 2011" by American Chemical Society, USA, and "Professor Suresh C Ameta Award, 2015" by the Indian Chemical Society, "Diamond Jubilee Professor for Life" by Karnatak University, Dharwad for his research contribution in the field of Chemistry, "Best Rotarian Award" by Rotary Club, Dharwad, 2021 for his distinguished service to mankind.

A dedicated academician, Professor Nandibewoor has contributed significantly to the development of research in the Country and also inspired a large number of students and colleagues who are carrying the torch of his mission.

The Indian Chemical Society sincerely wishes Professor Nandibewoor a long peaceful life with sound health and continuous academic activities for the advancement and propagation of Scientific Knowledge.

GDYadav

Professor G.D. Yadav
President
Indian Chemical Society

Chittaranjan Sinha

Professor Chittaranjan Sinha
Honorary Secretary
Indian Chemical Society

Acharya P C Ray Memorial Award Lecture

Prof. Prashant V. Kamat

How Semiconductor Nanostructures are Transforming Next Generation Photovoltaics

Prashant V. Kamat

Radiation Laboratory, Department of Chemistry & Biochemistry

University of Notre Dame, Notre Dame, IN 46556

Semiconductor nanostructures with tunable photoresponse can capture the visible and near IR photons quite effectively. By controlling the size and composition one can tune the photoresponse of semiconductor nanostructures in the entire visible region. The key advantage of semiconductor nanostructures lies in designing thin film solar cells with low temperature processing. These advantages significantly decrease the energy payback time since less energy is consumed (and hence a lower carbon footprint) during their manufacture.

The early studies which focused on the synthesis of semiconductor quantum dots and elucidation of charge carrier dynamics have led to the evolution of high efficiency metal halide perovskite solar cells. In the present talk light induced charge carrier generation and transport across interfaces which are important in the operation of solar cells will be discussed. Recent developments in utilizing semiconductor quantum dots in light energy conversion will be discussed.

Additional Readings

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[4] DuBose, J. T.; Kamat, P. V., Energy Versus Electron Transfer: Managing Excited-State Interactions in Perovskite Nanocrystal–Molecular Hybrids. Chemical Reviews 2022, 122, 15, 12475–12494

[5] Kamat, P. V.; Kuno, M., Halide Ion Migration in Perovskite Nanocrystals and Nanostructures. Accounts of Chemical Research **2021**, 54 (3), 520-531.

Biography

Prashant V. Kamat Prashant V. Kamat is a Rev. John A. Zahm, C.S.C., Professor of Science in the Department of Chemistry and Biochemistry and Radiation Laboratory at the University of Notre Dame. He is also a Concurrent Professor in the Department of Chemical and Biomolecular Engineering. Professor Kamat has for more than three decades worked to build bridges between physical chemistry and material science to develop advanced nanomaterials that promise cleaner and more efficient light energy conversion. He has published more than 500 scientific papers that have been well recognized by the scientific community Thomson-Reuters has featured him as one of the most cited researchers each year since 2014 (2014 -2022). He is currently serving as the Editor-in-Chief of *ACS Energy Letters*.

Acharya J C Ghosh Memorial Award Lecture

Prof. Amitava Patra

Exciting Nanomaterials for Photonic and Optoelectronics

Amitava Patra
Institute of Nano Science and Technology, Knowledge City, Sector 81, Mohali 140306, India
School of Materials Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India
Email: amitavapatra.patra@gmail.com, amitava@inst.ac.in

Nanomaterials-based light-harvesting systems have been the subject of research because they can generate exciton after photoexcitation. Here, we focus on the understanding of the exciton dynamics, energy transfer, antenna effect, charge carrier dynamics, and other related processes of 2D nanoplatelets, perovskite nanocrystals, conjugated polymer nanoparticles, metal clusters, and C-dots, and hybrid nanostructures.[1-8] Ultrafast spectroscopic investigations provide direct insight into the impacts of electron and hole transfer at the interface in the hybrid materials for optoelectronic applications. The fundamental knowledge of these photophysical processes is crucial for the development of efficient light-harvesting systems.

References

1. Simanta Kundu and Amitava Patra, Chem. Rev., 2017, 117, 712−757.

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3. Avisek Dutta, Anusri Medda, Soubhik Ghosh, Sumanta Sain, and Amitava Patra, ACS Appl. Nano Mater. 2022, 5, 11679−11688.

4. Subarna Maity, Sarita Kolay, Srijon Ghosh, Sikta Chakraborty, Dipankar Bain and Amitava Patra, J. Phys. Chem. Lett. 2022, 13, 5581−5588

5. Kritiman Marjit, Goutam Ghosh, Raju K Biswas, Srijon Ghosh, Swapan K Pati and Amitava Patra, J. Phys. Chem. Lett. 2022, 13, 5431−5440

Prof. Amitava Patra

Bio-Sketch

About Speaker: Prof. Amitava Patra is currently Director at the Institute of Nano Science and Technology (INST), Mohali, and a Senior Professor at the Indian Association for the Cultivation of Science. He was born in 1965 and received his Ph. D (1993) from Jadavpur University, India. Amitava pioneered the study of two-photon spectroscopy and ultrafast carrier dynamics on the contemporary topic of 2D structures, carbon dots, metal clusters, polymeric nanoparticles, and quantum dots for light-harvesting applications. We are interested to learn the mechanisms for photo-initiated processes such as exciton dynamics, ultrafast carrier dynamics, electron transfer, and energy transfer of nanomaterials for solar energy conversion. He is the author or co-author of more than 249 scientific papers, 5 book chapters, and 2 Indian patents. He was an Advisory board member of Nanoscale, Journal of Physical Chemistry, and others.

Prof. Amitava Patra is amongst the world's top 2% scientists in 2020 with a global rank of 149 in Physical Chemistry (Ranking is based on C-score). Prof. Amitava Patra has been elected as a Fellow of the Optical Society of America (OSA), and the Royal Society of Chemistry (FRSC). He is a Fellow of the Indian Academy of Sciences (FASc), India, and the National Academy of Sciences (FNASc), India. He is the recipient of National Prizes for Research in Chemical Spectroscopy and Molecular Structure, MRSI-ICSC Materials Science Annual Prize, C.N.R. Rao National Prize for Chemical Research, DAE-SRC Outstanding Investigator Award, A.V. Rama Rao Foundation Prize in Chemistry, AsiaNANO 2010 Award, CRSI Bronze Medal, Ramanujan Fellowship, MRSI Medal. His research papers have been cited more than 11800 by peers (h-index= 58).

Professor J N Mukherjee Memorial Award Lecture

Prof. K.K. Chattopadhyay

Graphene sheets, edges, quantum dots and some of their exciting attributes

Prof. K.K. Chattopadhyay
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The rise of graphene and other 2D materials can be attributed to their diverse ranges of electronic and optical properties favorable for many device applications. The fact that these 2D materials provide immense flexibility to tune its electronic properties at the atomic scale ushered a new era for material research. Among the many distinct features of graphene and rGO, changes in the peripheral edge site geometry, functionalization etc. and stacking with other 2D materials bear a significant effect on its electronic and optical properties.

It is a challenging task to fabricate hierarchical nanostructures of graphene or van der Waal stacked heterostructures and its controlled alignment for enhancing some of its properties for some specific applications. In this talk some of our results on the fabrication of aligned rGO sheets on nanostructured platforms, use of non-uniform electric field for alignment and also fabrication of hierarchical rGO will be discussed. Fabrication of quantum sheets of rGO and its functionalization for creating tailored luminescence will be presented. Density functional theory based calculation could reveal the origin of the observed tunable photoluminescence property [1-7]. Tailoring of other 2D materials and their composites for energy related applications will also be discussed.

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Professor Kankan Bhattacharyya Memorial Award Lecture

Prof. Anindya Datta

Spectroscopic insights into intermolecular interactions in protein-based biomaterials: In respectful memory of Professor Kankan Bhattacharyya

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Prof. Kankan Bhattacharyya was a stalwart, whose recognition and impact transcends boundaries, geographical and scientific. His path-breaking experiments on the dynamics of interactions in complex microenvironments, ranging from surfactant assemblies to live cells, continue to inspire researchers worldwide Prof. Bhattacharyya strongly believed that the essence of research is to seek answers to questions that no one asked before. This conviction remained the defining factor in all that he did, throughout his illustrious career. In reverence to the spirit and conviction that defined his research philosophy, two examples from our recent experiments on complex systems by time resolved fluorescence spectroscopy will be discussed in the present talk. The first of these is a study of dynamics of intriguing “water-less” protein liquids, which are self-assembled complexes of the cationized protein with the polymer surfactant (PS) glycolic acid ethoxylate lauryl ether.[1] The question we have asked here is whether such a system, practically devoid of water, exhibits slow solvation, associated classically with biological water, which fascinated Prof. Bhattacharyya.[2] In the second study,[3] dimethyl-2,5-bis[4-(methoxyphenyl)amino] terephthalate (DBMPT) has been shown to exhibit aggregation-induced enhancement of emission with Tween 40 and formation of nanorods with strong orange fluorescence. These nanorods disrupt fibrils of human serum albumin and lead to partial refolding of the protein. The resultant milieu emits white light, the mechanism of which has been explored. It is established that direct excitation of the acceptor plays a significant role, even though Förster resonance energy transfer (FRET) is found to be operative to some extent. A decrease in the fluorescence intensity and lifetime of ThT with progressive addition of DBMPT, which is often used as the sole indicator of FRET, is ascribed to the disruption of the fibrils by the nanorods. Once again, this is a problem that would resonate well with Prof. Bhattacharyya, who firmly believed that one cannot infer the operation of FRET, unless a risetime in the acceptor emission was observed.

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Prof. Anindya Datta

Bio-Sketch

Prof. Anindya Datta is presently working as Professor in Department of Chemistry, IIT Bombay. He obtained his Ph. D. from Jadavpur University in 1998. He was a postdoctoral fellow in Department of Chemistry, Iowa State University, USA and Visiting Scientist in Raja Ramanna Center for Advanced Technology, Indore, India. Prof. Datta's research is on ultrafast processes in molecules and materials. His group has studied the microenvironment of excited nafion membranes by excited state proton transfer of fluorescent probes. Anomalous pholoIuminescence of silica nanoparticles and light harvesting in silica-dye nanoconjugates has been another area of interest. In the last decade or so, the group has explored mechanisms of enhancement of fluorescence in fluorogenic molecules. Very recently, they have started exploring exciton dynamics in exotic photoluminescent nanocrystals, especially those that are dispersible in water. Prof. Datta is a Fellow of National Academy of Science, India and has received the Bronze Medal of Chemical Research Society of India. He serves on the Editorial Advisory Board of the Journal of Physical Chemistry.

Professor A. S. R. Anjaneyulu 60th Birth Day Commemoration Award Lecture

Prof. E. Balaraman

Our Odyssey with Dehydrogenation Chemistry for Sustainable Development

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Abstract:

Energy storage and the use of abundantly available feedstocks without contributing to the carbon footprint are the two main issues of this global challenge. In this regard, meeting the energy demand of the current society while avoiding environmental pollution requires the development of high-performance, low-cost, and environmentally-friendly sustainable catalytic systems. Our research interest at IISER-Tirupati includes the mechanistic approach to catalyst design for various important reactions with the aid of organometallic, nano, and photo(redox) catalysis for both fundamental research and industrial applications. Specifically, we work on the design and development of catalysts/catalytic materials based on non-precious metals for sustainable and affordable chemical synthesis from feedstocks *via* dehydrogenation chemistry,[1] hydrogen generation from renewables, and CO_2-based circular catalysis. *We also invested heavily in the development of electron donors for the Ziegler-Natta olefin polymerization catalysis.*[2]

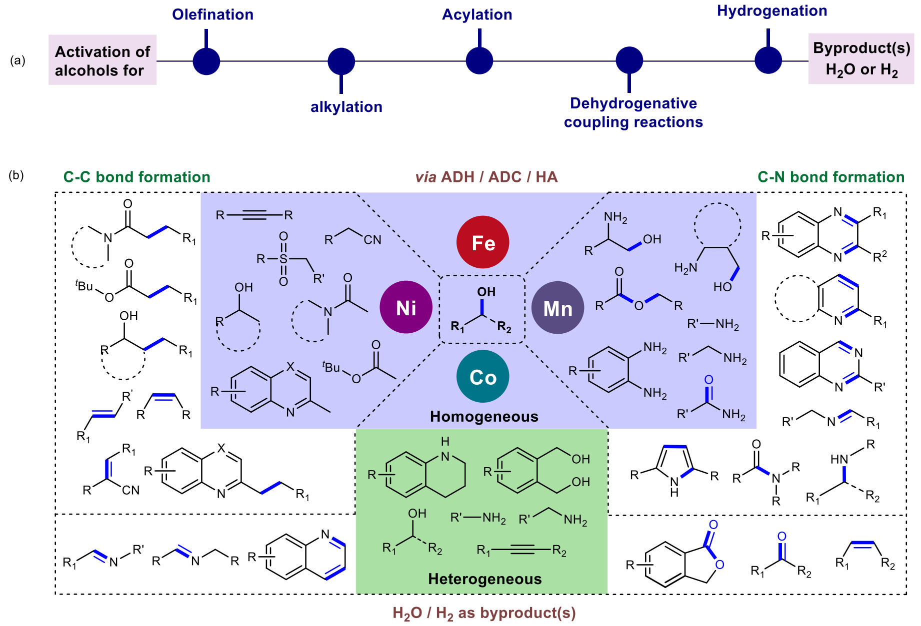

Figure 1. (a) Alcohols as feedstocks and (b) Sustainable chemical synthesis *via* dehydrogenation strategy using our approach.

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Professor Suresh C. Ameta Award Lecture

Prof. Sadhana S. Rayalu

Engineered Materials for Environmental and Energy related applications

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Environmental Materials Division, CSIR-National Environmental Engineering Research Institute (CSIR-NEERI), Nehru Marg, Nagpur- 440 020
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Abstract:

Materials and Catalytic chemistry is proving to be an essential prime requisite for making cleaner environment a reality and enhancing sustainability and carbon balance. Design of “engineered materials” for selective sorption and catalysis has been undertaken to meet the related growing environmental and energy challenges. A wide array of materials including nanostructured photocatalyst, biocatalyst, selective adsorbents and high energy materials have been developed for promising applications as illustrated below:

I)Energy related applications and Systems

- **i)** Hybrid and photocatalytic processes for solar hydrogen
- **ii)** Hybrid Materials for carbon capture and sequestration
- iii) New functional photothermal material and molecules for solar appliances and products

II)Environmental remediation

- iv) Reduced emissions firecrackers or green crackers
- v) Materials /product for menstrual waste management

Thus, application of engineered materials for SDG goals including affordable and clean energy and water, CCVS and solar hydrogen powered technologies for fuel cells shall be covered in the lecture.

Published work of Rayalu

(i) Throwing light on Platinized Carbon nano structured composite for hydrogen generation; Energy and Environmental Science, 2014, ***7****, 4087-4094;*

(ii) Photocatalytic water splitting on Au/TiO_2 nanocomposites synthesized through various routes: Enhancement in photocatalytic activity due to SPR effect; Applied Catalysis B; Environmental 142, 684-693, 2013;

(iii)Orthorhombic/cubic Cd2So4 Nanojunctions: enhancing solar water splitting efficiency by the suppression of charge recombination; Journal of Materials Chemistry; A 2 (2), 492-499., 2014.

Dr. (Mrs.) Sadhana Rayalu is Scientist & Head, Environmental Materials division of National Environmental Engineering Research Institute (CSIR), Nehru Marg, Nagpur. She is spearheading the research related to materials and catalysis in the area of energy and environmental technologies. She is leading the team of "green crackers" and has made significant contributions in developing new formulations with reduced emissions and also contributing towards related legal and policy interventions. She has to her credit around 170 SCI publications and 100 other publications. She also has more than 35 patents to her credit for technologies/process know-hows of industrial and societal relevance in following areas:

i) Plasmonic material-based composites developed for addressing "energy and environment nexus" issues (successful field demonstration of carbon capture & valorisation & solar energy triggered disinfection & distillation)

ii) **Functional and energetic materials** for Pyrotechnic compositions in specific for **Green crackers** with minimal emissions of particulate matter and gases (technology transferred to more than 1000 fireworks manufacturers)

iii) Functional materials developed for "**Broad band absorption cell (BBC)** in first of its kind hybrid photocatalysed water electrolysis system for generation of "Green hydrogen"

iv) **Functional materials for environmental catalysis including c**atalysts/materials for defluoridation of water and wastewater and air pollution control

She is coordinating various bilateral international programmes / collaborations including Indo-Korean, Indo-UK collaborations, Indo-US and has also visited these collaborating institutes. She has worked with multinationals like ALCOA, Horizon fuel cell and several industries in India including NOCIL, Rudraksh chemicals, NTPC, IRA agrotech etc. She has supervised the PhD thesis of more than 30 students. She has to her credit best paper presentation awards and other local and institutional awards for material development including CSIR technology award for green firecrackers, Vasvik and Chemcon award to name a few.

Professor S. S. Sandhu Award Lecture

Prof. Santi M. Mandal

Controlling Bacterial Pathogens Resistant to Antibiotics

Santi M. Mandal

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Antimicrobial resistance (AMR) is a major public health issue in terms of death and economic loss. It is extremely important to develop new classes of antibiotic with distinct activities, differ from traditional antibiotics. Antimicrobial peptides (AMP) are an alternate option because of their adjustable action by altering amino acid composition, amphipathicity, and charge. We tried multiple times to locate naturally existing AMPs and create a peptide-based structural analysis to increase activity. The structure-function connection of AMPs and heterocyclic complexes were examined in vitro to ex vivo. The role of efflux pump gene mutation and protein expression dysregulation are also critical characteristics in MDR strains, the development of efflux pump inhibitor is another strategy to halt them. Thus, combined effort on searching or synthesis of novel antibiotics, efflux pump inhibitors and thorough research on the genetic basis of antibiotic resistance should be the future answer to combat the antibiotic resistance pathogens.

Dr. G. Srivastava Memorial Award Lecture

Prof. Ajayan Vinu

Nanoporous materials with different functional elements: unique materials with multiple functions

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Abstract:

Nonporous materials with different functional elements are at the forefront in energy storage and conversion and environmental applications owing to their excellent photocatalytic and textural properties. 1-6 In the first part of the talk, I will present about different ways of preparing a series of nanoporous materials with different chemical framework elements including carbons, carbon nitrides, boron nitrides and boron carbon nitrides, fullerenes and heteropoly acids with different structures, morphologies and pore diameters. I will also present how these materials will be effectively used for solving the global issues including carbon capture and conversion and the clean energy generation including hydrogen production using visible sunlight. Much focus will be given on the fabrication of mesoporous carbon nitrides with different molecular structures and nitrogen contents and their performances in energy storage and conversion, hydrogen production and oxygen reduction reaction. The change in the molecular structure of carbon nitride materials has significant impact on the final band gap and the basic properties which influence their performance in photocatalysis and energy storage.

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Prof. Ajayan Vinu

Bio-Sketch

Prof. Vinu is currently working as a Global Innovation Chair Professor and Director of Global Innovative Center for Advanced Nanomaterials at the University of Newcastle and made a significant contribution in the field of nanoporous materials and their application in energy storage, fuel cells, carbon capture and conversion, hydrogen technologies, catalysis and drug delivery. His contribution has led to ca. 480 papers with 27,800 citations and a H-index of 85, and more than 32 patents. He has been ranked number 1 (last 20 years) and number 7th (last 50 years) in Australia among the Top 2% scientists in the field of "Materials" as per the database created by the Stanford University in 2020, reflecting his high-quality research and research impact that he made in this field. The quality of his research has been recognised with several international awards including Medal, Chemical Research Society of India 2018, SPARC award 2019, CNR Rao Lectureship award 2019. Medal and KY NIEM CHUONG Award 2018, Scopus Young Researcher Award 2014, Friedrich Wilhelm Bessel award by the Humboldt Society (2010), JSPS Senior Invitational Fellow 2014, Australian Future Fellowship 2010, Indian Society for Chemists and Biologists award for excellence 2010, Catalysis Society of India Young Scientist award 2010, Chemical Society of Japan Award for the Young Scientist 2008, and Laureate of Khwarizmi International Award 2008. Prof. Vinu is honoured with the Fellow of Royal Society of Chemistry, RACI, World Academy of Ceramics, World Academy of Art and Science, Indian Chemical Society, and Asia-pacific Academy of Materials.

Professor R. D. Desai 80th Birthday Commemoration Award Lecture

Prof. Sagar Pal

Biopolymeric flocculants: Development and applications

Sagar Pal

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Abstract:

Recently in authors' laboratory, various functionalized biopolymeric flocculants have been developed through simple modification of natural biopolymers. The synthesised flocculants demonstrated excellent efficiency towards reduction of pollutant content from mine process water at Industrial scale[1], showed outstanding efficacy towards selective recovery of high-quality Fe-ore particles from the mixture of inorganic gangues[2-3]. These developed products are economically viable, easy to synthesize and are worthy to be used in real industrial applications.

References:

1. *Indian Patent No. – 378107* (Date of Grant – 28.09.**2021**)
2. *Indian Patent Application No*. 201631037148, **2016**.
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Prof. Sagar Pal

Bio-Sketch

Prof. Sagar Pal is currently working as Professor in the Department of Chemistry and Chemical Biology, Indian Institute of Technology (ISM) Dhanbad. He is also Dean (Research & Development) of the Institute. He is a Fellow of the Royal Society of Chemistry and Indian Chemical Society. He was also the recipient of the DAAD Fellowship 2012. He is also the Council Member, The International Council on Materials Education, USA. He has 21 years of research experience in the field of polymer chemistry. His research focus is on the development of polymeric biomaterials/polymeric gels/polymeric micelles/polymeric flocculants and their potential applications in various fields. He has guided 13 PhD students, and presently 5 more students are pursuing their PhD under his direct supervision. He has been credited with 92 International publications, 8 Review articles and 8 patents (out of which 2 patents have been granted) with an h-index of 43 and citations more than 5800.

Rev. Fr. L. M. Yeddanapally Memorial Award

Prof. Deepak Chopra

Cocrystallization: A Design Element in the Applications of Organic Solids

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Abstract:

The method of co-crystallization involves the design *via* the principles of crystal engineering, prediction *via* machine learning and synthesis of new crystalline phases, wherein the properties of the new phase are different from those of the individual components [1]. This technique has been applied in the design of new drugs with improved physico-chemical properties [2]. In particular charge-transfer (CT) cocrystals, have found applications as photoluminescent materials [3], dielectrics [4] and as triboelectric nanogenerators (TENGs [5]).

The talk will discuss the design, synthesis, crystallization and a mechanistic understanding of the role of CT cocrystals as dielectrics [4]. Furthermore, these have also been fabricated into devices and find applications as TENGs [5].

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Prof. Deepak Chopra

Bio-Sketch

Dr. Deepak Chopra is currently a Professor in the Department of Chemistry at Indian Institute of Science Education and Research (IISER) Bhopal, Madhya Pradesh. He joined the Institute in March 2009. He received his degree in B.Sc. (H) Chemistry (Gold Medallist) from Jadavpur University in 2001. Following which he pursued the Integrated PhD program (which includes a 3-year MS program) from Indian Institute of Science (IISc), Bangalore in Chemical Crystallography under Prof T. N. Guru Row. He continued as a postdoctoral fellow in IISc till 2007. He further continued his postdoctoral work at the University of Toledo, Ohio, USA in the field of electron density analysis in molecular crystals under Prof Alan A. Pinkerton. His active research interests, includes investigation of polymorphism in drugs and pharmaceuticals, computational analysis of non-covalent interactions, *in situ* crystallization, experimental/theoretical electron density analysis and mechanical/electrical properties in molecular crystals. He is currently on the Editorial Board of *Journal of Molecular Structure*, Elsevier, and the RSC journal *CrystEngComm*, a Co-Editor of the journal *Acta Crystallographica E* (IUCr, Chester), a *Fellow* of the *Indian Chemical Society* (FICS) and a *Fellow* of the *Royal Society of Chemistry* (FRSC).

Professor Dhananjay Nasipuri Memorial Award Lecture

Prof. Alakesh Bisai

Nature Inspired Total Syntheses of Architecturally Complex Natural Products of Biological Relevance

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Abstract:

Nature produces a variety of complex natural products in entioenriched form (see, Figure).[1-2] Since these are isolated from Nature in limited quantity (mostly in mg scale), total synthesis endeavors can play a crucial role in bioactivity evaluation by providing access to significant quantity.[1-4] It also provides platform for the innovation of new strategies for chemical synthesis.[5-6] In this regard, naturally occurring alkaloids with impressive diversity of biological activities drew our interest.[1a] Interestingly, a variety of alkaloids of this family show interesting biological activities, such as antibacterial and cytotoxic activities.[1a] Towards this direction, we explored novel oxidative strategies under mild condition that will be discussed in this talk.[7]

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Prof. Alakesh Bisai

Bio-Sketch

Alakesh obtained his Ph.D. from IIT Kanpur in Sept. 2006 (Supervisor: Prof. Vinod K. Singh). Immediately afterward, he moved to the University of California, Berkeley, CA, where he held postdoctoral position with Prof. Richmond Sarpong (Sept. 2006 – Dec. 2009). During his stay at Berkeley, he completed the total synthesis of '*lycopodium alkaloids*' lyconadin A, that received considerable attention from the synthetic community. In Dec. 2009, he left Berkeley and joined Department of Chemistry, IISER Bhopal as an Assistant Professor of Chemistry, later he was promoted to an Associate Professor followed by Professor (Jan., 2018) and continued his Academic journey till May, 2020. Meanwhile, he moved to the Department of Chemical Sciences, IISER Kolkata in May, 2019. The research focus of the AB research group includes the total synthesis of architecturally interesting and biologically active natural products that provide an ideal platform for the invention of new strategies and highly selective organic transformations. His total synthesis has been highlighted in '*Organic Chemistry Portal*' as '*The Bisai Synthesis of (-)-Physovenine*'. The research of the AB Group has been appreciated in various forms, to name a few notable ones:

Prof. P K Bose Memorial Award Lecture

Prof. Jyotirmayee Dash

Nucleic Acid Directed Cycloaddition

Jyotirmayee Dash

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Indian Association for the Cultivation of Science, Kolkata

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Abstract:

DNA and RNA secondary structures play key regulatory roles in biological system. In this talk, nucleic acids directed synthesis of their small molecule binders will be described. DNA and RNA secondary structures have been used as templates to promote alkyne and azide cycloaddition in the absence of any metal catalysts. Non B-DNA structures like the four stranded G-quadruplexes and i-motifs have been used to synthesize carbazole based triazolyl ligands with promising anticancer properties. HIV-1 TAR RNA has also been used as a template to synthesize a peptidomimetic ligand. The *in situ* synthesis of ligands for biological targets is a potential approach to directly achieve bioactive small molecules by combining synthesis and screening steps.

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Prof. Jyotirmayee Dash

Bio-Sketch

Dr. Jyotirmayee Dash obtained her Ph.D. in Organic Chemistry from IIT Kanpur, India. She was awarded Alexander von Humboldt fellowship at Freie University, Berlin, a postdoctoral fellowship at ESPCI-Paris, and Marie Curie fellowship at University of Cambridge, UK. She first joined IISER, Kolkata as an Assistant Professor in 2009 and is currently working as a Senior Professor at IACS-Kolkata. She received DST Swarnajayanti (2015-2016) and DBT Wellcome Trust (2020) Fellowships and Shanti Swarup Bhatnagar Prize (2020). Her research interests include new organic transformations, structure and function of nucleic acid targets.

Award Lecture (Dr. Basudev Banerjee Awardee)

Prof. Goutam Brahmachari

Direct C-H functionalizations of coumarins under green-approach: a retrospection of our sincere efforts

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Abstract:

Coumarins (2-oxo-2*H*-1-benzopyrans) belong to an important class of potentially bioactive natural *O*-heterocycles and their synthetic versions. Such scaffolds were screened as building blocks in a plethora of organic transformations in the recent past. Coumarins, thus, offered the basic structural motifs of many potent drug candidates, including anticoagulants, antibiotics, antioxidants, anticancer drugs, antituberculosis drugs, anti-inflammatories, and many more. This group of compounds find uses as additives in foods and cosmetics, fragrances and perfumes, and agrochemicals. Such molecules find extensive applications also as fluorescent sensors, optical brighteners, fluorescent transthyretin folding sensors, and molecular photonic devices. The overall feasibility of synthesizing and/or functionalizing numerous valuable organic motifs largely depends upon the success of carbon-carbon and/or carbon-heteroatom bond formation. Direct C-H bond functionalization has recently attracted significant attention as an advantageous technique for constructing carbon-carbon and carbon-heteroatom bonds in modern synthetic chemistry. Under this purview and as part of our ongoing green chemistry research, we also screened such a potently bioactive coumarin moiety as the building block to design and synthesize various functionalized coumarin derivatives of biological relevance. A few of our selected synthetic drives in functionalizing coumarins to access novel series of *O*-heterocycles under green-approach will be presented in this meeting,

Related References

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Prof. Goutam Brahmachari

Bio-Sketch

Dr. Goutam Brahmachari is a full professor of organic chemistry at Visva-Bharati University, Santiniketan, India. The research interests of his group include organic synthesis, green chemistry and medicinal chemistry of natural and natural product-inspired synthetic molecules. With 24 years of experience in teaching and research, he has produced about 240 scientific publications, including original research papers, review articles, books, and invited book chapters in organic synthesis, green chemistry, and natural products. He has already authored/edited twenty-six (26) books and 50 book chapters from internationally reputed leading scientific publication houses, including Elsevier, Academic Press, Royal Society of Chemistry, Wiley-VCH, World Scientific, CRC Press (Taylor & Francis and others. He is the *Founder Series Editor* of the Elsevier Book Series, '*Natural Product Drug Discovery*'. Prof. Brahmachari is a Fellow of the Royal Society of Chemistry, and a recipient of *CRSI (Chemical Research Society of India) Bronze Medal-2021* (contributions to research in chemistry), *INSA (Indian National Science Academy) Teachers Award-2019*, *Dr. Kalam Best Teaching Faculty Award-2017*, and *Academic Brilliance Award-2015 (Excellence in Research)*. Prof. Brahmachari was featured in the World Ranking of the Top 2% Scientists (Organic Chemistry Category by Stanford University) in 2020, 2021 and 2022, and the AD Scientific Index 2022 World Ranking of Scientists -2022.

Prof. A. K. Chandra Memorial Award Lecture

Prof. Ayan Datta

Buckling and Defects in Two - Dimensional Atomically Thin Monolayers

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Graphene has emerged as one of the most fascinating areas of research in condensed matter and materials science. Apart from graphene, several other 2D analogues like silicene, phosphorene, MXenes, MoS_2, germanene have been recently isolated and characterized. One unifying theme among these new materials is that unlike graphene, they are non-planar. Pseudo Jahn-Teller (PJT) distortions is shown as a central unifying concept that explains the overall structural preferences of these systems. The extent of buckling also leads to interesting and emerging phenomenon like phase-transitions into Topological Insulators from normal semi-metal due to spin-orbital coupling (SOC). The effect of PJT in bestowing structural diversity and novel electronic and spin phases in 2D-monoatomic layers will be discussed in this lecture. How to utilize them for CO_2 conversion to useful chemicals will envisioned.

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Prof. Ayan Datta

Bio-Sketch

Prof. Ayan Datta, after his Ph.D. in 2007, worked as a postdoc in USA for a few years before starting his own independent group at IISER TVM. In 2012, he moved to IACS, and his group is working on the development of computational models for energy and environment. He is the recipient of the INSA Young scientist award and BM Birla Prize in Chemistry. He was also awarded the distinguished investigator award (DIA) by DST-SERB in 2017. He was awarded a Bronze medal by the Chemical Research Society of India (CRSI), India. He serves the Editorial Advisory Board of Journal of Physical Chemistry A, B and C of American Chemical Society.

Prof. Sankar Chandra Moi

Pt (II) based anticancer drug design and drug development

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National Institute of Technology Durgapur
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Abstract:

Heterocyclic or aliphatic diamine and sulfur containing amino acid chelated anticancer agents [1-3] of Pt(II) complexes $[Pt(Diam)Cl_2]$ C-1, $[Pt(Diam)(H_2O)_2]^{2+}$ C-2, [Pt(Diam)(L-cys)] C-3 and [Pt(Diam)(DL-meth)] C-4 (where, Diam = Diamines) were synthesized and characterized by spectroscopic methods. Kinetic investigation with bio- relevant molecules was investigated and their ‘Drug reservoir’ mechanisms are proposed from the calculated activation parameters ($\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$) and rate constants for both steps (k_1 & k_2). Theoretical investigation is also another part of this research work like; TD-DFT, NBO analysis and IRC. DNA and BSA binding activity of the complexes were investigated by UV-Vis and fluorescence spectroscopic methods. The molecular docking of complexes was performed to observe the interaction of the complexes with CT-DNA and BSA. In vitro BSA binding activity of the complexes was under consideration as model ‘drug reservoir’ and ‘transport medium’ for carrying Pt(II). Bio-physical[4] investigations like; conformational change of BSA in presence of drug candidates was studied by Förster resonance energy transfer (FRET) calculation, synchronous and 3D fluorescence spectroscopic study. Anticancer activity of the complexes was studied with Hep-G2, A-549 and normal cell lines and their IC_{50} values were compared with well-known anti-cancer drug cis-platin and other recognized drugs. ROS generation activity on normal cell also measured and compared with cisplatin, indicates better than traditional drug. Remarkably, all these complexes were tested by NBT assay on normal cell line skeletal muscle cells (L6 myotubes), which revealed that these complexes have minimum adverse effect compared to recognized anticancer medications. The aim is to explore the cell death mechanism for which cell cycle study has been performed by flow-cytometer with the complexes on HEp-2 cell lines.

Prof. Susanta Lahiri

Recent Trends in Nature Resourced Radioanalytical Chemistry

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Abstract:

The phrase Nature Resourced Chemistry was coined in 2019, which is a step forward in the purview of Green Chemistry. Nature resourced chemicals (NRC) are defined as the chemicals derived from nature and used in chemical processes. Recently we have proposed few radiopharmaceuticals with NRCs of different varieties like hesperidin derived from orange peels, caffeine and catechin derived from tea leaves, etc. In radioanalytical chemistry, minuscule amount of radioisotopes are used, therefore elucidation of structures of NRC- Metal complex is almost impossible by spectrometric techniques. The computational chemistry helps in this regard to understand the underlying chemistry.

Dr. Vishwanath Patil

Innovative approaches of nanomaterials for societal applications

Vishwanath Patil

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Abstract:

Nano-chemistry is a relatively young area of study dedicated to perfecting methods for creating materials on the nanometer scale (1–100 nm). Nanomaterials display unique features such as magnetic, electrical, optical, mechanical, and catalytic properties that are substantially different from their bulk counterparts. Nanomaterials' advantageous properties make them prime candidates for the design and preparation of novel functional materials with applications in a wide range of sectors, including catalysis, imaging, medicine, energy research, coatings, and the environment. Our research group demonstrated that the nanoparticles can be used for the invisible barcoding of carbon fiber and glass fiber-reinforced epoxy composite parts that are used in the manufacturing of airplanes, expensive luxury cars, and other automotive sectors. Based on nanotechnology we have developed multi-substrate Antiviral Nanocoating by in-situ production of copper and silver nanoparticles inside a polymer matrix that has antiviral capabilities to deactivate SARS-CoV-2 from contaminated surfaces to restrict further spreading effectively. These coatings are aqueous, but after film formation, they turn hydrophobic to provide strong water-resistant films with good washing fastness and long-lasting antiviral effects. Nanotechnology may also be employed to improve the lithium-ion battery' s electrochemical performance. In order to increase the value of recycling, we enhanced the electrochemical performance of recovered graphite throughout the recovery process to create a high-performance nanocomposite that could be utilized to produce innovative anode materials.

Keywords: Nanomaterials, Invisible barcoding, Antiviral Nanocoating, SARS-CoV-2

Prof. Alka Sharma

Engineered Nanostructured Materials for Sustainable Environment

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Abstract:

Today, eco-sustainability and energy are the prime issues standing in the midst of deep crisis and utmost need of the hour for the progress of civilization in the era of modern technology. Amongst the three pillars of sustainability (social, environmental and economic), eco-sustainability is the most vital to be concerned and nanotechnology is the only pivotal tool for eco-sustainability. In view of the eco-damaging factors involved with conventional methods (chemical/physical) of nanomaterial synthesis, the non-conventional (greener) approach is vividly advocated for the production of nanostructured materials. A variety of nanostructured materials have been synthesized via non-conventional route employing indigenous natural resource, weeds, invasive species, etc. which are richly constituted with bioactive phytochemicals which act as reductant, stabilizer and capping agent. Engineered nanostructured materials have proficiency to eradicate environmental toxicants/pollutants compared to bulk materials. A number of bulk materials showed astounding features when probed at nano scale. Engineered nanostructured materials play significant role in many sectors, viz., biomedical, pharmaceutical, life-sciences, catalysis, optics, solar cells, energy conversion, metal and other industries, etc. These have also been investigated for their efficacy as photocatalyst, corrosion-impeders, eradication of aquatic-pollutant, and many other noteworthy utilities. Fabricated nanostructured materials have been verified by carrying out characterization using standard tools and techniques, viz., FTIR, UV-vis, FL, AFM, SEM-EDS, XRD etc. The non-conventional approach has many advantages over conventional, as it is toxicant-free, eco-friendly, easier, economic, energy-saver, fast, and reliable. Consequently, the researchers ardently advocate, globally adopting the non- conventional (green) approach to fabricate nano-structured materials as remediation for sustainable environment. Over a decade, it has witnessed as a mile stone in conserving environment.

Dr. Ajit Joshi

Synthesis and Characterization of 5-Methylisoxazole Derivatives by LCMASS & ^{1}H-NMR Technique and Its Potentials Application

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Abstract:

The present disclosure of the invention presents a novel 5-methylisoxazole derivative & method of preparation thereof. These newly synthesized compounds were characterization and confirmation by LCMASS and ^{1}H-NMR Spectroscopy. These 5-methylisoxazole derivatives showing antibacterial, antifungal, and antimalarial activity, against the STD drugs. These compounds would be of better use in drug development to combat bacterial infections and as anti-malarial agents.

Prof. Kamlesh Shrivas

Inkjet-printed paper-based electrodes with gold nano-ink for electrochemical detection of glucose

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Raipur-492010

Abstract:

Herein, an inkjet-printed paper electrode (PPE) with gold nanoparticle (AuNP)-ink as a non-enzymatic electrochemical sensor for detection of glucose in blood serum is reported. In this work, a green method is used for the synthesis of the aqueous AuNP-ink. Herein, starch was used as a reducing as well as capping agent. The prepared AuNP-PPE was employed as a working electrode in cyclic voltammetry (CV) for the sensitive measurement of glucose in blood serum. The fabricated AuNP-PPE demonstrated excellent electrochemical activity and rapid electron transfer kinetics towards the oxidation of glucose. A wide linear range, 0.05–35 mM with a limit of detection of 10 µM is observed for the determination of glucose. There are several chemical species present in blood serum and their existence may affect the electrochemical properties of the AuNP-PPE for selective determination of glucose, which are referred to as interfering species. The advantages of using the AuNP-PPE in electrochemical measurements is flexible, user-friendly, biodegradable, economic and enzyme-free with respect to the commercially available electrochemical sensors.

Prof. Badal Kumar Mandal

Analytical techniques for separation and characterization of microplastics in environmental samples

Badal Kumar Mandal
Department of Chemistry, Vellore Institute of Technology (VIT)

Abstract:

The 2030 UN Sustainable Development Goals include “ensure sustainable consumption and production patterns, with emphasis on preventing, reducing, recycling and reusing” plastics and other products [1]. Microplastics (1µm to 500 µm) with high specific surface area for sorption of contaminants and high penetration potential in the bodies of organisms might be a concern to all stakeholders. In addition, the existence of complex matrices in soil, biological, and wastewater samples poses a critical challenge to the analysts for the separation of microplastics in identifying and quantifying by using different analytical tools. Different separation techniques such as density-based, hydrophobicity-based, size-based, solubility-based, polarity-based chromatography, electrostatic and magnetism-based, and thermogravimetric-based approaches are adopted for the separation of microplastics. The major challenge in this process is to remove complex matrices from the environmental samples without degrading, corroding, melting, or deformation of the microplastics. In this paper, the associated separation techniques and different analytical tools are assessed for separation followed by their characterization.

- 1 year as a CSIR research associate at Jadavpur University (1998-99)
- 2 years (2000-02) at Chiba University-Japan (as JSPS Fellow)
- 2 years (2002-2004) at the National Institute of Radiological Sciences-Chiba, Japan (as STA cum JSPS Fellow).
- 1 year (2005-2006) at the University of Texas at San Antonio as a research scientist
- 120 international and 30 national research articles in different journals.
- More than 50 refereed conference proceedings
- 13 book chapters, and one research investigation report with Toyo Chemicals Company Ltd.-Japan on arsenic calamity in India and the possibility of removal plant
- Completed 3 DST projects
- 12 students have received Ph.D. degrees under Dr. Mandal’s supervision on nanomaterials, drug delivery, method validation, and clinical trials
- Dr. Mandal has guided 50 M.Sc. and M.Tech. theses
- Presently, six more Ph.D. students are doing research under his supervision
- Dr. Mandal has one Indian Patent (Patent No: 283985 dt.6/6/17).
- Dr. Mandal is concentrating research works on the toxicity of metal and metal oxide nanoparticles as well as their composites, the remediation of toxic heavy metals using metal nanoparticles and carbon-based nanocomposites, and sensing of heavy metals using electroanalytical techniques

Prof. Subhashis Roy

Chemical Approaches Toward Eco-friendly and Stable of Perovskite Based Thin Films Solar Cells

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Abstract:

The present research deals with the advancement of thin film-based perovskite solar cells by considering the most crucial factors, including degradation, instability, and toxicity, which are undesirable for perovskite photovoltaic technology. In this research work, we have successfully fabricated lead (Pb)-replaced and Pb-free perovskite solar cells at ambient conditions and developed a new fabrication route for highly efficient and air-stable perovskite solar cells. The carcinogenic Pb has been replaced by non-toxic tin (Sn) at ambient conditions under excess chlorine (Cl)-rich system to minimize the degradation tendency of Pb-free perovskite solar cells. The Pb-replaced perovskite solar cells have been further annealed at different annealing conditions to investigate the effect of annealing temperatures on the photovoltaic performances, which led to the formation of nanostructured-perovskite solar cells. The investigation showed that the construction of nanostructures is a function of annealing temperatures. The thermal engineering study under an excess Cl-rich system has shown positive influences on the stability, surface morphology, structural crystallinity, optical properties, and photovoltaic performance of Pb-replaced perovskite solar cells. The density functional theory (DFT) was also performed to investigate the electron distribution phenomenon for Pb-free and Pb-replaced perovskite solar cells. The thermal engineering study has influenced to develop a new fabrication route called the dual-step thermal engineering technique for developing a highly-efficient and stable methylammonium lead iodide (CH 3 NH 3 PbI 3) based perovskite solar cells at ambient conditions. The detailed investigation has shown that the newly developed dual- step thermal engineering technique is potential over the conventional one-step spin coating method as the new method exhibited remarkable improvement in the efficiency and stability of perovskite solar cells. All the perovskite thin films and photovoltaic devices were extensively explored by different characterization techniques and Rietveld refinement simulation study using FullProf Software to understand the fundamentals of perovskite's crystalline structure.

Dr. Subhasis Roy is working as Assistant Professor at Department of Chemical Engineering, University of Calcutta, India. Dr. Roy received Ph.D. from Indian Institute of Technology, Kharagpur. Before joining as a faculty member at Calcutta University, he worked as a Postdoctoral Researcher at Sungkyunkwan University, South Korea, Research Scientist at IISER, Kolkata, and worked as a visiting researcher Raman Fellow, Ohio University. Dr. Roy has published more than 65 scientific research papers in peer-reviewed journals, 20 conference publications. He has 18 book chapters, edited 2 books and filed several patents. Dr. Roy was awarded DST-Fast Track Young Scientist Start-Up Research Grant from SERB – DST, Mission innovation MI IC#5' DBT-DST joint funding grant, Teachers Associateship for Research Excellence (TARE) SERB –DST. He holds membership of many professional societies such as Royal Society of Chemistry (MRSC), National Academy of Sciences, India (NASI) and reviewers as well as editorial board member of many international journals. His expertise is in perovskite solar cells, multiferroic composite thin films, photocatalysts for water splitting, fuel cells, and hydrogen energy.

Prof. Neelima Gupta

Multi-target Binding Profiles of Therapeutic Agents with Biomolecules

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University of Rajasthan, Jaipur-302004

Abstract:

Investigation of the drug-biomolecule interactions occupies an important domain in modern drug discovery process. Drugs interact with biological molecules via a variety of mechanisms, which is the basis for particular therapeutic effect of a drug candidate. Drug repurposing is becoming an effective means to find new therapeutic applications of known drug candidates due to their multi-target affinities. There are several analytical strategies available to understand such interactions between therapeutic agent and biological receptor. Spectroscopic techniques such as UV, Fluorescence and CD are useful to estimate the strength of interactions experimentally. Some of these methods have been utilized to provide an estimate of the overall binding along with stoichiometric assessment of drug-receptor complex. Besides, computational approaches such as Docking, MD and QM-MM calculations have also been applied to study effectively the structural aspects of these complexes. Computational tools have provided structural information in terms of position and orientation of in the receptor pockets along with their binding free energy values. Results from our recent investigations of the multi-target binding profile of anticancer agents with DNA and HSA in a dynamic physiological environment using spectroscopic, molecular dynamics simulations, and quantum mechanical calculations to evaluate the structural features, mode, ligand, and receptor flexibility and energetics of complexation will be presented.

Neelima Gupta after obtaining her M.Sc. (Chemistry) degree in 1987 from Kurukshetra University, joined University of Rajasthan, Jaipur as a NET-JRF to pursue her Ph.D. degree in synthetic organic chemistry under the supervision of Prof. R.K. Bansal. After completion of her Ph.D. in 1992, she served as Lecturer in a Government College for two years and subsequently worked as a Postdoctoral fellow sponsored by German Research Foundation at the EMA University of Greifswald, Germany, prior to joining the University of Rajasthan as Assistant Professor in 1996. She progressed there as Associate Professor (2006) and Professor (2012). She has held the responsibilities of the Coordinator, UGC-Center of Advanced Study in Chemistry and currently, holds the position of Director, PG School of Physical Sciences and Addl. Director at Centre for Converging Technologies at University of Rajasthan. She started her research in computational chemistry under DST's fast-track project for young scientists (2002) and later was also a visiting scientist to the Computational Chemistry Group in Phillips University of Marburg under Indo-German cooperation program. Her research interests vary from low coordinated phosphorus chemistry, synthetic heterocyclic chemistry to computational chemistry assisted study of reaction mechanism and drug-biomolecule interactions. Dr. Gupta has completed several research projects, supervised 14 Ph.D. students, has more than 80 Research Publications in International Journals of repute and one Patent to her credit. She has authored chapters in international reference series - Science of Synthesis (Thieme Chemistry), Topics in Heterocyclic Chemistry (Springer-Verlag) and Methods in Pharmacology and Toxicology (Springer-Verlag). In 2009, she was awarded for Excellence in research among Top Researchers of the University of Rajasthan. Dr. Gupta has received "ISCB-Distinguished Women Scientist Award–2019." As one of the founding Conveners of the CRSI-Rajasthan Chapter, she is actively engaged in Chemistry popularization program and is also Secretary in Chemical Research Society of India's present governing council. She has organized several National and International Conferences and delivered more than fifty invited talks in National and International conferences, symposiums, workshops in India and abroad.

Dr. Nimai Chand Pramanik

Dev. of Supercapacitors and its Accepted Test Protocols for Applications in High-Power Electronics

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Abstract:

Self-reliance on ‘Energy’, particularly the energy storage & transmission under ‘Atmanirvar Bharat’ is one of the important thrust of area of research in India. Accordingly, Govt. of India has taken several initiatives towards the development of efficiently sustainable, eco-friendly and cost-effective technologies on Energy storage to fulfill various national missions on energy, such as National Solar Mission, National Clean-energy Mission, National Electric Mobility Mission, etc., which also would be capable in reduction of carbon foot print and emission of green-house gases. Development of high-power, high energy density Supercapacitors (SC) are most relevant towards the fulfilment of country’s Electric Mobility Mission. By virtue, supercapacitors are highly capable of storing of large amount of electric charges/energies rapidly that can also be delivered to the loads at faster rates. In addition, because of fast charge-discharge characteristics with high usable capacitance, ultra-low ESR, longer cycle-life and wide ranges of operating temperatures, supercapacitors are of high demands in automobile and power-electronic sectors, where because of inherent slow charge-discharge characteristics of LiB (Li-ion batteries) and similar other battery based systems alone are inadequate. In this context, development & fabrication of SCs, especially for applications in high-power systems, say EV/HEV and other power-intensive electronics is a great challenge and considering the need & demands, it has immense R&D potentials. Researchers in India and abroad have intensive R&D and reported potentiality of various carbonaceous and non-carbonaceous materials, such as CNT, GNF, aerogel carbon (AGC), activated charcoals, biomass derived carbons (AC), conducting polymers, transition metal oxides (say, Ru2O, MnO2, NiO, Co3O4, etc.) for use as active material for SCs. However, activated carbons (AC) and aerogel based porous 3D nanostructured carbons (AGC) exhibited the most suitability in making high-power supercapacitors and AC only was explored commercially.

Flexible screen printed immunosensor for electrochemical detection of small cell lung cancer

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Abstract:

Neuron-specific enolase (NSE) is a putative serum marker for SCLC with the normal range of 15 ngmL-1 in healthy adult’s serum, and elevates up to around 25 ngmL-1 in patients with SCLC. [1] [2] Moreover it has been recognized as a potential clinical marker for covid-19 because coronavirus primarily targets human respiratory and neurological system.[3] Electrochemical techniques in conjugation with immunosensor are of great interest for detection of NSE due to its potential efficacy as specific, simple, label free rapid analysis as well as point care detection (POCT).[4] Despite of substantial advancements, the substrate modification procedure is still laborious and challenging. In this context, we have explored a **porous organic polymer Polymelamine formaldehyde (PMF)** as an efficient substrate material on **paper-based screen-printed electrode for label free** detection of NSE.The purposed immunosensor has achieved the wide detection range of 120 fM-70 nM (9.4 pg/ml - 5.5 µg/ml) with tail on orientation of antibodies without the assistance of any coupling as well as blocking agent for early diagnosis of small cell lung cancer.

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Eco-Friendly MoS2 Nanosheets Encapsulated by PVA Capped Mn doped ZnS Nanoparticle Sensor for Electro Sensing of Carcinogenic *p*-Dimethylamino Antipyrine.

*Manjunath B. Megalamani a and Sharanappa T. Nandibewoor *a*
a Department of Chemistry, School of Advanced Sciences, KLE Technological University, Hubballi-580031, Karnataka, India.

Abstract:

p-Dimethylamino Antipyrine (*p*-DAAP), is an agranulocytosis causing carcinogen. In this study electrode for the analysis of *p*-DAAP was utilized by PVA capped Mn dopped ZnS encapsulated through MoS2 nanosheets on glassy carbon electrode. Characterization was performed using XRD, SEM-EDX and FTIR. Electrochemical impedance spectroscopy (EIS) was used to study the material's performance. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) have been utilized to assess *p*-DAAP, under different phosphate buffer solutions, the *p*-DAAP demonstrates an oxidation and a reduction peak, with pH 6.0 demonstrating the best outcome. The impact of various factors on electrochemical properties was investigated, demonstrating the diffusion electrode process. The DPV is utilized to do quantitative assessment. The linearity field was between 0.2 µM -16µM. The LOD and LOQ have been 1.08 x 10-8 M and 3.60 x 10-8 M respectively. The novel method was employed to evaluate the concentrations of *p*-DAAP in biological and water samples.

Application of silver nanoparticles as sensing probe for colorimetric and paper-based detection of riboflavin (B2)

Tikeshwari and Prof. Kamlesh Kumar Shrivas
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Abstract:

We report plasmonic colorimetric and paper-based sensor for selective detection of riboflavin (B2) using silver nanoparticles (AgNPs) modified with polyvinyl alcohol (PVA) as a sensing probe. The plasmonic colorimetric sensing based on red shift of localized surface Plasmon resonance (LSPR) in UV-Vis region from 405 to 445 nm and paper based exploited the color change of AgNPs from yellow to yellowish red that is fabricated on paper substrate. The paper-based detection use of smartphone for recording the change of color after the vegetable/fruit samples on test region of paper fabricated with AgNPs and change in color intensity is determined by color detector app. The mechanism for selectivity for determination of B2 is experimentally validated by performing UV-Vis, Fourier transforms infrared spectroscopy (FTIR), transmission electron microscope (TEM), and dynamic light scattering (DLS) measurement. Finally, the plasmonic colorimetric and paper-based sensor were successfully applied for analysis of B2 in vegetable and fruit samples. The results of paper-based detection were validated by Plasmon colorimetric and TEM analysis determination of B2 in real sample.

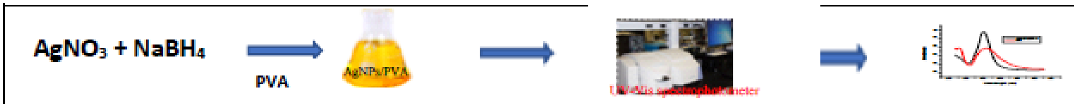

Fig: - Procedure for colorimetric (UV-Vis spectrophotometric) detection of vitamin B_2 using AgNPs as a nanoprobe

Reference:

Kamlesh Shrivas, Monisha, Tushar Kant, Indrapal Karbhal, Ramsingh Kurrey, Bhuneshwari Sahu, Deepak Sinha, Goutam Kumar Patra, Manas Kanti Deb & Shamsh Pervez, Smartphone coupled with paper-based chemical sensor for on-site determination of iron (III) in environmental and biological samples, Analytical and Bioanalytical Chemistry volume 412, pages1573–1583 (2020).

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Evaluation of the Synergetic rheological behaviour of polymer and Silica Nanofluids for Enhanced Oil Recovery

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Abstract:

Nanoparticles (NPs) are employed in various petroleum exploration and production technologies, including drilling, well logging, reservoir management, and enhanced oil recovery (EOR). The petroleum industry has high hopes for the increased oil recovery potential from Silica nanofluids, which are stable mixes of nanoscale particles distributed in base fluids. The dispersion of NPs in the aqueous polymer solution was characterized by DLS and zeta-potential measurements for stability. In the rheological studies, it was observed that there was an improvement in the viscosity by adding Silica Nanoparticles in polymeric solution. The experimental results showed that Silica Core flooding experiments were performed to observe the synergetic efficacy of the nanofluids with polymer in sandstone cores of different permeabilities at 90°C. Thus, it can be said that these Silica Nanofluids can reduce the contact angle and improve the viscosity of the polymeric solution, resulting in the enhancement of oil recovery.

Investigation of Fluid/Fluid interactions of Green Nano-emulsion for Enhanced Oil Recovery in Petroleum Reservoirs

Chirag Bhadiyadra, Rohit Kumar Saw, Ajay Mandal*

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Abstract

Researchers have formulated Nano-emulsion using n-Alkanes hydrocarbons as the oleic phase that is non-biodegradable in nature. The present work deals with the formulation of Nano-emulsions using two nonionic surfactant (Tween 40 and 80) and methyl Ester (formulated using vegetable oil) for application in enhanced oil recovery. Green Nano-emulsion developed using Ester as an oleic phase is biodegradable and environment friendly. Nano-emulsions were formulated by High energy method and stability studies were conducted by bottle test at a wide range of temperatures (30, 50 and 70 °C) and time. Formulated Nano-emulsions were found to be highly kinetic stable with a zeta potential of around -33 mV and droplet size in the range between 59 to 150 nm. IFT values were found to decrease significantly with surfactant concentration and temperature. Formulated Nano-emulsions were found to have higher viscosity than the plain surfactant solution showing higher mobility control required for enhanced oil recovery.

Keywords: Nano-Emulsions, Surfactants, Ester, Rheology, Enhanced Oil Recovery.

Synthesis and Application of Natural Surfactant derived from olive oil for Enhanced Oil Recovery from Sandstone Reservoirs

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Abstract:

Applications of natural surfactants have become an important area of study in recent years because of environmental consequences of conventional surfactants used in petroleum upstream. In this study, a non-ionic surfactant has been synthesized from Olive oil via two step reaction procedure. Formation of synthesized surfactant was confirmed through FTIR analysis. Synthesized surfactant showed promising properties of emulsification and rock wettability alteration. Results indicated that synthesized surfactant has a very low critical micelle concentration (CMC). Emulsification studies were carried at CMC with varying salinities to screen out the optimum salinity showing WINSOR-III phase. Contact angle test confirmed the optimum salinity results showing excellent wettability alteration capability of surfactant. The loss of surfactant by adsorption on the rock surface was also studied, and the adsorption data were analyzed by different adsorption isotherms. Above results showed that synthesized surfactant has good capability for the application in enhanced oil recovery in sandstone reservoirs.

Keywords: Natural Surfactants, Olive oil, Emulsification, Wettability alteration, Enhanced Oil Recovery.

Prof. C. M. Reddy

Crystal engineering of adaptive smart materials

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Abstract:

High crystallinity, although desired in materials for a wide range of high-performance engineering applications, generally comes with undesirable attributes such as high brittleness and fragility [1]. This makes crystalline materials incompatible with many future technologies, such as flexible devices and soft-robotics. Recent progress in crystal engineering has brought into light many possible opportunities to address these issues, enabling the design of adaptive crystalline materials that respond to external stimuli with exceptional qualities [1-7]. For instance, crystals that bend (elastically or plastically), twist, curl, wind, jump, exfoliate, laminate, and explode, under external stresses, such as mechanical stress, pressure, light, heat, solvent, etc., have been shown. On the other hand, until very recent time, self-healing was observed only in soft and amorphous materials, mostly involving approaches that use chemical reactions, diffusion, solvent, vapour, electricity, etc., with typical healing time scales in minutes to weeks [8]. A new self-healing mechanism that we recently introduced [9] in materials science, enables ultrafast, near 100% autonomous diffusion-less repair in crystalline materials that uses electrostatic surface potentials generated on the freshly created fracture surfaces, inherent to certain types of polar single crystals. My talk will cover structure-property correlation for crystal engineering of adaptive materials.

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Dr C. Malla Reddy is currently a Professor and Head at the Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata. Dr Reddy has graduated in Crystal Engineering from University of Hyderabad. He has been awarded with the prestigious Swarnajayanti Fellowship in Chemical Sciences for the year 2015, by the Department of Science and Technology, Government of India. He has published over 100 peer-reviewed research articles. Currently, he is serving as an Associate Editor for CrystEngComm by RSC and co-editor for Acta Crystallographic Section B.

His research group at IISER Kolkata focuses on establishing a structure-mechanical property correlation for designing various functional solids using crystal engineering principles. His group is credited for pioneering work on mechanically flexible molecular crystals and self-healing single crystals of piezoelectric molecular materials.

Dr. Basudev Pradhan

Progress and Challenges in the Development of Next Generation Solar Cells Technology

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(GEET), Central University of Jharkhand, Ranchi, India.
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Abstract:

The energy crisis is becoming one of the most critical issues all over the world these days. In every year, the global energy demand increases continuously, especially the developing country like ours have a huge shortage of electricity. However, fossil fuels are limited, thought to run out and are held responsible for increased concentration of carbon dioxide in the earth's atmosphere, which causes global warming. The consequences of the effect are already seen as an increase in the frequency and severity of natural disasters. The use of nuclear power as an energy source is not accepted by the wide section of the world population anymore because of security and health risks. Furthermost, the disposal of nuclear waste is still an unsolved problem worldwide. These drew the attention to urgently develop environment friendly renewable energy sources. One of the renewable energy sources is photovoltaic (PV) technology, which generates electricity directly from solar radiation. The photovoltaic cells have become extensively studied since the 1950s when the first crystalline silicon solar cell, which had an efficiency of 6%, was developed at Bell Laboratories. Since then, the efficiency has reached 26.1% for crystalline Si solar cells, which is already close to the theoretical predicted upper limit of 31%. Today's photovoltaic modules are extremely safe and reliable products, with minimal failure rates and projected service lifetimes of 20 to 30 years. Due to the high cost of crystalline silicon solar cells, different emerging new- generation solar cells like organic solar cells, perovskite solar cells, and Quantum dot solar cells are down the line to take over the PV market. Recently, the solution-processed organic tandem photovoltaic cell has achieved a record 17.3 % efficiency. The perovskite solar cells are also one of the most promising PV technologies, which has achieved 25.7 % efficiency in single cell structures in just over 12 years of R&D research all over the world. If the stability issues of perovskite solar cells are solved then it will be the first next generation solar PV technology, which will be commercialized very soon with very low production cost compared to conventional crystalline silicon solar cells.

Dr. Basudev Pradhan is an Assistant Professor, Department of Energy Engineering, and Centre of Excellence (CoE) in Green and Efficient Energy Technology (GEET) in the Central University of Jharkhand, Ranchi, Jharkhand. He received his PhD from Indian Association for the Cultivation of Science (IACS) and Jadavpur University, India. He was Alexander von Humboldt research fellow in Germany for 2010-12, Ramanujan fellow funded by DST for 2013-2018, and BASE fellow at University of Central Florida funded by IUSSTF. He spent more than four and half years as a postdoctoral fellow at Arizona State University, University of Wisconsin-Milwaukee, University of Surrey, and University of Potsdam. His research interests focus on perovskite solar cells, organic solar cells, and Nanoelectronic devices etc. He has published 40 high quality research papers in the reputed international journals and one edited book. He has 3 US patents (1 granted). He is one of the associate editors in Applied Physics A, Springer Nature journal since 2014

Dr. Debasis Banerjee

Catalytic (De)-hydrogenations of Alcohols and Diols: Sustainable Strategies to Bioactive *N*-heterocycles

Debasis Banerjee

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Abstract:

N-heterocycles are most valuable compounds ubiquitous in bioactive molecules, alkaloids, and extensively used in pharmaceuticals, agrochemicals and as ligands.[1] Therefore, inter or intramolecular catalytic selective C–N and C-C bond formation for their synthesis is an ultimate goal in chemical research. Conventional methodologies for their synthesis involve multi-step pathways and suffer from low atom economy, limited selectivity and produced stoichiometric amounts of waste.[1] Direct application of renewable alcohols or diols as electrophilic coupling partner represents a sustainable alternative, as they can be readily available in industrial scale production from lignocellulose biomass.[1]

Recently, there is a potential drive to replace precious noble-metal catalysts using earth abundant and inexpensive non-noble metals for sustainable organic transformations. Since past couple of years, we have developed the applications of non-precious metal-based catalysts for such transformations using hydrogen borrowing catalysis. We have demonstrated a general and practical applications of various primary alcohols, including diols and amino alcohols for selective construction of numerous five or six-membered *N*-heterocycles. Our recent studies on the de-hydrogenation technologies for one-pot synthesis of bio-active pyrroles, pyridines, indoles, imidazoles etc. will be discussed. A detailed mechanistic and kinetics studies were also established for such transformations.[2-6]

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Debasis Banerjee graduated with M.Sc. degree in Organic Chemistry from Banaras Hindu University and obtained Ph.D. in organic chemistry from Indian Institute of Technology Kanpur in 2011 with Prof. M. L. N. Rao. Thereafter he moved to Leibniz Institute for Catalysis (LIKAT), Germany for a postdoctoral position with Prof. Matthias Beller (2011-14) and subsequently held another postdoctoral position (2014-2015) at the Stockholm University, Sweden with Prof. Jan-Erling Bäckvall. In 2015, he has accepted a position of Assistant Professor at the Indian Institute of Technology Roorkee (Uttarakhand, India). Currently he is an Associate Professor at the same institute from August 2020.

Research Interests:

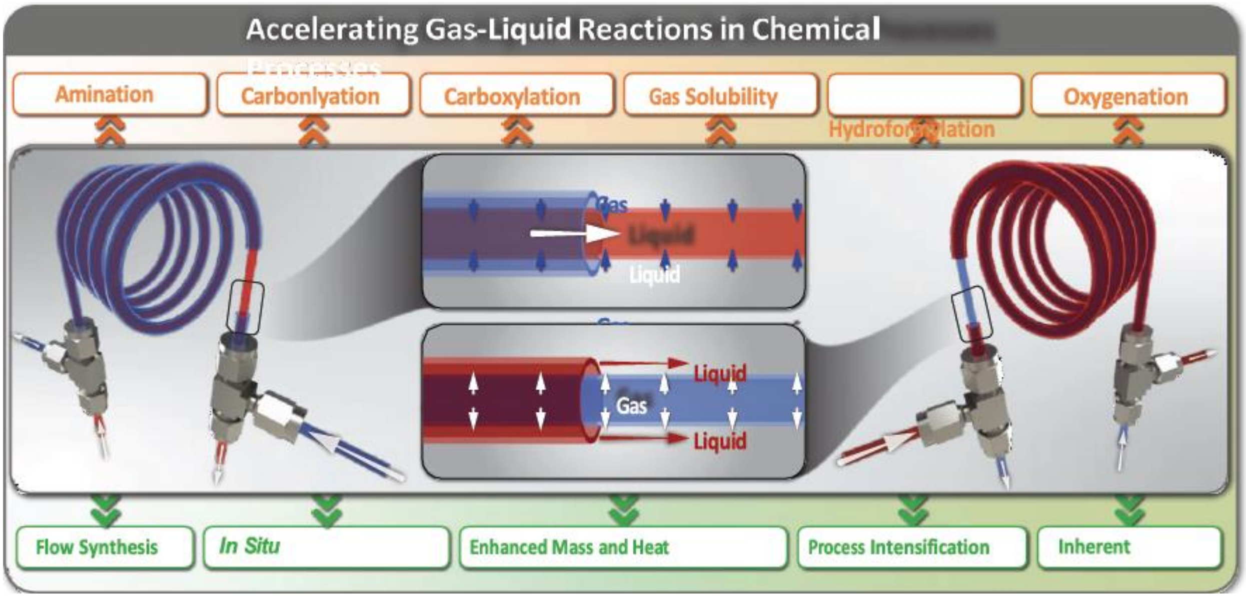
Redox-switchable catalysis (RSC) relates to tuning the catalytic activity of a transition metal by designing a suitable ligand in combination with more abundant non-precious metals, enantioselective dual-catalysis, activation of small molecules, perfluoroalkylation technologies and heterogeneous catalysis for sustainable organic transformations.

Awards and Honours:

He is a recipient of SERB-Early Career Research Award (2016), DAE-Young Scientist Research Award (YSRA-2016) and winner of Evonik Call for Research Proposal (ECRP-2016) Award by Evonik Industries GMBH, Germany. Recently has been selected for the Thieme Chemistry Journals Award 2020. Since 2021 he is working as a Guest Editor in *Tetrahedron* and *Tetrahedron Letters* on a Special Issue based on Non-Precious Metal-Catalysis for Sustainable Organic Transformations. He has been selected for the Chemical Research Society of India (CRSI) Bronze Medal of 2023.

Dr. Keshav Raghuvanshi

Continuous Manufacturing of Heterocycles via Flow Chemical Technology



Abstract:

At issue are heterocycles, which change their biological activities when exposed to active binding substrates. However, from an industrial perspective, there are significant challenges. Specifically, continuous flow chemical manufacturing can determine the acceleration in as little as screening.

Dr. Sharad Lande

Industrial Catalysis for Green Processes & Sustainability

Dr. Sharad Lande

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Abstract:

The challenge of moving toward a greener and more sustainable society will inevitably require the drastic transformation of many aspects of modern culture and economy. Green chemistry is built upon advances in areas and disciplines that existed prior to the field's inception including catalysis, atom-economical synthesis, waste minimization, and circular economy. Catalysis plays a vital role in the environmentally benign synthesis of new and existing chemicals.

Petroleum and petrochemical industries have revolutionized our life and are providing the major basic needs of rapidly growing, expanding and highly technical civilization as a source of energy for domestic, industrial, transport sectors and as feedstock for fertilizers, synthetic fibers, synthetic rubbers, polymers, intermediates, explosives, agrochemicals, dyes, and paints etc.

Heterogeneously catalyzed processes constitute the basis for a large number of chemical technologies employed nowadays. The use of materials such as: Al_2O_3, SiO_2, TiO_2, Zeolites and supported metal catalysts among others, has a rich history of success in the production of industrial catalysts which are used for development of green processes. The present talk will discuss about impact of industrial catalysis, green processes, sustainability, concept to commercialization stages, challenges, and future opportunities.

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Dr. Sharad Lande did Ph.D. in Chemistry (Recipient of Gujarat Ambuja Cement best Ph.D. thesis award 2005) from ICT (UDCT) Mumbai with Padma Shri Prof. G.D. Yadav. He did Post Doctorate research at University of Ottawa, Canada for 2 years. He joined Reliance in 2007 and currently working as AVP(R&D) at RIL, Mumbai. He has more than 20 years of research experience in the field of heterogeneous catalysis, Adsorptive purification, Nanomaterials for VOCs removal & CO_2 Purification. He has significantly contributed for 8 technologies development commercialized from lab scale to commercial scale & 7 on pilot scale which are ready for commercialization. 53 patents filed in various countries and out of which 15 granted in India & abroad, 55 international & conference publications.

Recent Awards/Honours:

- Elected as a Fellow of Royal Society of Chemistry, London, UK, 2022;
- Winner- CII Industrial Innovation Awards 2021 for commercialization of in-house developed Catalyst& Adsorbents;
- Performance Excellence Award in Leadership 2021 by Global Education & Corporate Leadership (GECL-2021);
- Elected as a Fellow of Indian Chemical Society 2021;
- National Distinguished Researcher Award 2021, by the International Institute of organized Research;
- Selected Finalist for International Hydrocarbon Processing 2021 Award for Best Petrochemical Technology for adsorptive process;
- Selected as Member of CII National Committee on Technology, R&D & Innovation 2022-23.

Dr. Indu Bhushan Deb

Electrosynthesis and Spiro-annulations: Direct Access to Nitrogen-Containing Heterocycles

Indu Bhusan Deb
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Abstract:

Organic electrosynthesis is an inherently environmentally benign technique as it uses the electron as a redox agent instead of sacrificial hazardous chemical oxidants or reductants as in traditional chemistry. As such, electrosynthesis does not produce waste. Electron transfer can occur against a potential gradient, allowing for electrolysis at lower potentials and reducing the undesired side reactions. The ubiquitousness of dibenzoxazepines, benzazepines, benzoxazine, benzosultam, quinazolines, indoles, acridines and tetrahydroquinolines in various natural products and pharmaceuticals make them immensely valuable heterocycles. Hence, the development of a new and efficient method for their synthesis and derivatization assumes high significance. Recently, we have developed several efficient and mild methodologies via direct and selective C-H functionalization employing the concept of electrochemical, metal-catalyzed spiro-annulation and hydride shift reactions for the synthesis of densely functionalized potential bioactive heterocycles. This basic and fundamental research directed us to develop cost-effective processes for the synthesis of commercially available drug molecules including tropisetron and tilorone. Which will be discussed during the presentation.

Publications:

1. **PATENT:** 0163NF2021, 202111047806. **PCT**/IN2022/050940, 20 Oct, **2022.**
2. **PATENT:** 0211NF2020; 202111047809. **PCT**/IN2022/050931, 19 Oct, **2022.**
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5. Deb, I. *et al.* ***Org. Lett.* 2021,** 23, 4521-4526 (IF 6.091)
6. Deb, I. *et al.* ***J. Org. Chem.* 2021,** 86, 4131-4142 (4.335).
7. Deb, I. *et al.* ***Adv. Syn. & Catal.* 2021,** 363, 826-832 (5.851).
8. Deb, I. *et al.* ***Org. Lett.* 2020,** 22, 1340-1344 (IF 6.091).
9. Deb, I. *et al.* ***Org. Lett.* 2019,** 21, 2056-2059 (IF 6.091).

Dr. Indu Bhusan Deb obtained his M.Sc. degree in organic chemistry from Banaras Hindu University. He completed his Ph.D in 2008 at the Indian Institute of Technology Bombay (IITB) under the supervision of Professor I. N. N. Namboothiri. Thereafter, he moved to Rutgers University, USA to carryout postdoctoral research with Professor Daniel Seidel where he was involved in doing research for the synthesis of chiral heterocycles. After spending three years at Rutgers, he joined in the group of Professor Naohiko Yoshikai at Nanyang Technological University, Singapore, for his 2nd postdoctoral research. In April, 2013 He joined as a research investigator (Project leader) in process chemistry division of Bristol-Myers Squibb Research center in Bangalore. Dr. Deb worked as a senior scientist in the division of Organic and Medicinal Chemistry at CSIR-IICB, (Jan, 2014-2018). At present, Dr. Deb is Principal scientist and associate Professor (AcSIR) in the same division. His research group is actively involved in asymmetric synthesis and designing synthetic methodology employing transition metal–catalyzed C-H bond activation chemistry, metal-free reaction and Organo-electrosynthesis for the synthesis of potential bioactive small molecules.

Dr. Amiya Priyam

Soft Chemical Routes to Tunable Plasmonic and Luminescent Nanocrystals for Catalytic and Therapeutic Applications

Amiya Priyam

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Abstract:

The advent of nanotechnology has brought new solutions to the pressing problems in the society and is improving the quality of life for the mankind. However, most of the nano-syntheses utilize capping agents, reducing agents and solvents that are damaging to the environment. There is a need to make the processes greener and cleaner. The talk describes the aqueous syntheses routes for plasmonic and luminescent nanomaterials using mild reagents and under normal temperature and pressures. In the first part, synthesis of hollow plasmonic nanoshells of silver is described which have tunable size, shape and structure. Application of such nansostructures in solar-catalysis and chemo-photothermal therapy will also be discussed. The choice of silver stems from the fact that it has highest quality factor for surface plasmons and greater photothermal efficiency in the spectral region of 400-1200 nm. Thus, it presents an opportunity to study the plasmonic properties over wide wavelength region and harness them for suitable applications.

Hollow silver nanoshells (HAgNS) with tunable plasmon bands were synthesized by employing a combination of mild reductant (hydrazine hydrate) and a mild stabilizer (sodium citrate). The plasmon peak was tuned in a wide range from 460 nm to 630 nm. In the second part, we also developed a method using folic acid as stabilizer. A peculiar folate-directed shape transformation from solid nanospheres to hollow silver nanocubes (HAgNCs) has also been discovered and temporal evolution was spectroscopically followed.

The cube-shaped hollow silver nanoshells were found to be very good solar photocatalyst in the entire visible range at sub-picomolar level. These hollow silver nanocubes Furthermore, the Anisotropic Silver NCs vis-à-vis spherical have been found to act as an excellent SERS tool for the detection of metal ion contaminants such as of As (III), Cr (III) and Cr(VI).

Among the soft approaches for luminescent NCs, A supersaturation-controlled synthesis of ZnTe QDs was developed and their non-linear optical properties have been investigated by the Z-scan technique using a low power He-Ne laser (15mW, 632.8 nm) in a non-resonant condition. The ZnTe QDs having an average size of 0.8 nm and 1.7 nm followed the three-photon absorption model. The QDs were well-suited for the fabrication of all-optical switching devices. The self-assembled nanostructures also offer themselves as an attractive alternative to conventional materials in making waveguides for SCG application.

Dr. Mir Wasim Raja

PAPERATOR: The next generation sustainable Paper based Separator for LIBs and Supercapacitors

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Abstract:

India recently reviewed its energy policy and proposed a road map under a program called "National Mission for Electric Mobility". To reach the designed milestones, rechargeable batteries, particularly Lithium-ion Batteries are going to play a significant role due to its higher energy density and power density. India requires about 50-gigawatt hour (GWh) of battery storage capacity over the next two-and-a-half years to support the projected growth in renewable energy sector and also to meet the estimated demand electric mobility (EVs/HEVs). In parallel, the "Atmanirbhar Bharat" initiated by GOI has also triggered an extensive R&D effort for developing indigenized rechargeable battery technology such as Lithium-ion Batteries (LIBs) or its equivalent low-cost Na-ion Batteries (NIBs). To start manufacturing these batteries in India, all its components such as anode, cathode, electrolyte, separator, metal can, metal films, etc. are need to be produced locally. With this aim, CGCRI is actively persuading different research activities on developing cost competitive and value-added battery components.

Since 2016, CCGRI is engaged in developing cellulose based paper separator which can replace the existing plastic polyolefin based costly PP/PE commercial separator membrane due to its problem related to the severe dimensional shrinkage at elevated temperature, poor electrolyte wettability and safety. Recently CGCRI successfully developed paper based ceramic separator (named as "Paperator") which showed excellent electrolyte wettability (>200%), negligible shrinkage at high temperature (~250°C), high chemical stability in cell environment, quicker saturation time w.r.t electrolyte and comparable electrochemical performance to that of PP/PE separator. CGCRI also developed an environment friendly aqueous based paper separator fabrication process and installed a double-decker in-situ temperature-controlled fabricating machine designed in-house. Under a recent research initiative to develop electrolyte component, CGCRI is exploring the possibilities of developing novel fast Li-ion conducting garnet electrolyte-based separator cum electrolyte membrane- a step towards development of PAPER CELL technology.

Dr. Wasim currently working as Senior Scientist in Energy Materials and Devices Division (EMDD) at CSIR-CGCRI, Kolkata. He completed his M.Sc. degree in Physical Chemistry from University of Burdwan and received his Ph.D. from Jadavpur University, Kolkata in the year 2010 in area of high-performance electrode materials for Lithium-ion battery (LIBs) technology. After completion his Ph.D., he served as Assistant Manager (R&D) in UNTPL, Indo-US JV limited company dedicatedly working on production of nanostructured electrode materials for LIBs in India. In 2012, he joined as Senior Scientific Officer in Chemistry Division in State Forensic Science Laboratory, Kolkata, Govt. of West Bengal and served till 2020. At Forensic Lab he established a new Management Division in 2017 and was leading a group of 16 scientific personnel for R&D in forensic sciences. He has been honored as guest faculty and National trainer for future safety and failure investigation of high-end vehicles by LNJN-NICFS, MHA, New Delhi.

During his stay at battery industry, he is supervising bulk production of electrode materials, fabrication of 18650 LIB technology and application of LIBs for Mines, Solar storage, Mobile tower powering energy banks etc. Dr Wasim received MRSI-Young Scientists award (Kolkata Chapter) in 2007 for his contribution in engineered microstructures for high performance battery materials. He published 17 research papers in SCI journals, presented more than 22 research articles in National/International conferences on batteries. He patented 6 technology related to synthesis of battery grade electrode materials and paper based ceramic separators.

Currently, at CGCRI, he is actively working on developing low-cost paper based ceramic separators and Monolithic All Solid-State Lithium Batteries (MASSLB). His broad area of research consists of metal-ion batteries, Solid State batteries, synthesis and bulk scale production of engineered battery grade electrode powders, applications of LIB packs and lithium battery system integration.

Synthesis of copper loaded surfactant-modified chitosan beads for catalytic reduction of 4-nitrophenol

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b Civil Engineering Department, Indian Institute of Technology Kharagpur, Kharagpur-721302, India
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Abstract:

Chitosan hydrogel (CS) beads are modified with sodium dodecyl sulfate at a concentration higher than critical micelle concentration to form surfactant-modified chitosan hydrogel (SMCS) beads. The CS and SMCS beads are used to remove Cu(II) from water. The waste Cu(II)-loaded CS and SMCS beads, designated as Cu-CS and Cu-SMCS, respectively are further used as a catalyst for the reduction of 4-nitrophenol (4-NP) to 4-aminophenol (4-AP) in aqueous NaBH4 which is an approach towards zero-waste management. As the Cu(II) loading on SMCS is similar to that of CS beads so the catalytic efficiency of Cu-CS and Cu- SMCS in the reduction of 4-NP to 4-AP is compared. The zero-order rate constant of Cu-SMCS at a dose of 0.2 g/L is found as ~30 times higher than Cu-CS which is due to the synergistic effect of the surfactant bilayer on the surface of Cu-SMCS. Thus, waste Cu-SMCS proves to be an efficient catalyst.

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Study of the Catalytic Activity, Structural and Microstructural Properties of Mn0.3Zn0.7Fe2O4 Microspheres Synthesized by Solvothermal Method

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Abstract:

Herein we report structural and microstructural properties along with the catalytic activity of the micro-structured solid spheres of Mn0.3Zn0.7Fe2O4 synthesized [1,2] by one-pot solvothermal method. Powder x-ray diffraction, field emission scanning and high-resolution transmission electron microscopic together with energy dispersive x-ray spectroscopic (EDS) techniques are employed to systematically investigate its structural and microstructural properties. The above-mentioned studies reveal that the sample is a single-phase mixed spinel ferrite of $Fd\bar{3}m$ space-group and it is solid microspheres having average diameter ~421 nm constituted with nanoparticles (~ 21 nm). The EDS spectrum of the sample confirms that its constituent cations are present in proper stoichiometric ratio. Interestingly, the sample exhibits very good catalytic response towards degradation of Congo Red under dark condition, which is very rare. [2]. The degradation efficiency of the sample reaches a maximum 138% at 90 minutes. Thus, it can be used for industrial waste water treatment.

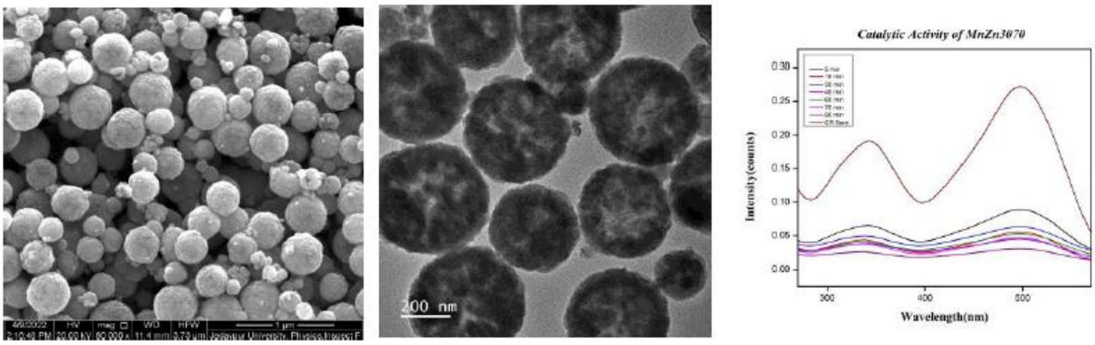

Fig: FESEM image, HRTEM image and catalytic activity of $Mn_{0.3}Zn_{0.7}Fe_2O_4$ solid microsphere

References:

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Chitosan based Mesoporous Silica Nanohybrids for Antibacterial, Antioxidant and Drug Delivery Applications

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Abstract:

The encapsulation of chitosan biopolymer onto functionalized silica surfaces to obtain organically modified nanohybrid is a great challenge to the researchers. From this objective the present work will focus on mesoporous silica modified chitosan nanohybrids for antibacterial, antioxidant and drug delivery applications. Here we have reported thiol modified chitosan-silica, chitosan succinate–g-amine functionalized mesoporous silica, aminosilane@mesoporous silica/ chitosan@salicylaldehyde (MSN@NH_2/CS@SCA) hybrids for above studies. The prepared nanohybrids were well characterized and showed particle sizes around 200nm, zeta potential around -19.0±6.0 mV for surface charges, and durability which suggested that they can be used to enhance their biological activities like antibacterial, and antioxidant. Quercetin drug release behavior of nanohybrids in PBS solution (72 h) at pH-5.0: 57, 69 and 76 % respectively and at pH-7.4: 29, 23, and 20% respectively. The antibacterial and antioxidant activities are also found in the enhanced ranges.

Keywords: Chitosan, mesoporous silica, antibacterial, antioxidant , drug delivery.

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Design and Development of Oxindole Based Anti-cancer Therapautics And its Bioapplication.

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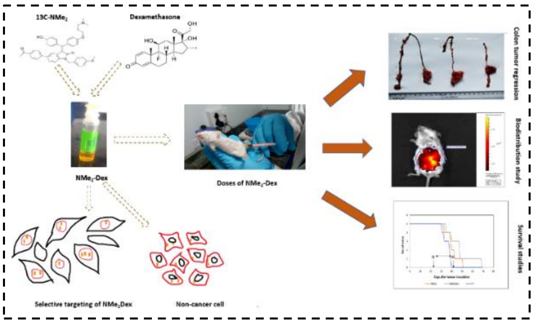
Abstract:

Oxindoles, as previously studied are used as potent anticancer agent having many relevant biological properties and this class of molecule has contributed immensely in the field of medicinal chemistry. The most important feature of oxindole is that it can be modified into various novel structures which are not only be used as anticancer agents but also can be used as antifungal, antimicrobial agents as well as for treating neurodegenerative diseases. Our previously developed bis-arylidene oxindole, NMe_2 exhibits effective targeting towards estrogen receptor-positive (ER+) cells. Herein, we designed a new analogue of NMe_2, called 13C-NMe_2 exhibiting structural resemblance with tamoxifen, an ER antagonist. Understandably, the concept of targeting ER is limited to ER+ cancer cells, while it leaves no scope for targeting other cancers. Additionally, caution must be exercised as ER is expressed in both cancer and non-cancer cells. In here, we found that 13C-NMe_2 can self-aggregate in aqueous solution and hence besides exhibiting its own anticancer property, it shows the capacity to carry within it other drugs. This self-aggregative property of 13C-NMe_2 repurposed this molecule to treat other cancers. Co-formulating glucocorticoid receptor (GR) synthetic ligand, dexamethasone (Dex), 13C-NMe_2 aggregate could target and kill ER (-) colorectal cancer cells also. Elucidating the mechanistic aspect of anticancer property of the Dex-associated aggregate (NMe_2-Dex), we find that NMe2-Dex induced ROS and apoptosis by affecting mitochondrial pathways. The cell cycle study further illustrated that the cells are being arrested in G2/M phase thus reducing cancer cell proliferation. Moreover, *in vivo* orthotopic colorectal tumor model studies revealed that NMe_2-Dex treated group has a better survivability along with a better tumor regression. Additionally, NMe2-Dex showed sensitization and killing of colorectal cancer cells can be a better therapeutic approach towards selective targeting and because it has an aggregative property, this gives an additive or synergistic killing effect on colorectal cancer cells. Moreover, the aggregative property of NMe_2 renders it to have a lipophilic and hydrophobic balance. This property makes it unique to act as a delivery system with a targeting ligand.



Co-formulation of NMe_2 -Dex and its selectivity towards colorectal cancer

Gold- Nanoparticle/ Carbon Quantum Dots Composites: Synthesis, Characterization and Applications

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Abstract:

Nano-composites are new generation of nano-materials (NMs). Nanocomposites are multiphase materials in which one phase is observed to be dispersed onto another phase, consequently, having the combination of individual properties of both the component materials [1]. In this work, we have reported a simple, cost-effective, and rapid synthesis procedure for the synthesis of gold-NPs / carbon quantum dots (AuNPs/CQDs) composite by chemical reduction method. Firstly, CQDs have been synthesized by hydrothermal method using Poly-(ethylene glycol) as carbon precursor and then auric chloride added at appropriate amount to synthesize AuNPs/CQDs composite. The synthesized AuNPs/CQDs composite have been characterized by fluorescence Spectroscopy, UV-visible spectroscopy and FTIR spectroscopy. Further, the synthesized AuNPs/CQDs composite may be successfully applied to fabricate a sensor for the detection purpose.

Keywords: Nano-composites, Gold-nanoparticle/ carbon quantum dots, toxic substance.

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Detection of antibiotic using natural pigment- surfactant- drug as ternary system

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Abstract:

In this work we have developed fluorescent sensor for the aminoglycosidic antibiotic drug, based on the aggregation induced emission enhancement (AIEE) fluorescence using natural pigment and surfactant ternary system.[1] The fluorescence spectra of natural pigment is quenched in aqueous medium due to its aggregation, which is further recovered in the presence of anionic surfactant i.e., sodiumdodecylsulphate(SDS). The fluorescent intensity of quenched pigment is also recovered with addition of ciprofloxacin drug .The fluorescence of natural pigment is enhanced due to its solubilization in drug-surfactant aggregate of *natural pigment-surfactant-analyte* system[2].This work formulates way for development of selective sensing methods.

Keywords: anionic surfactant, fluorescent, natural pigment, antibiotic drug.

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Simultaneous determination of several water-soluble vitamins in green leafy vegetables using reverse phase-high performance liquid chromatography

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Abstract

A simple, quick, and competent RP-HPLC-DAD method is optimized for quantitative determination of several water-soluble vitamins in green leafy vegetables. A gradient program was developed for separation of vitamins using 20 mM phosphate buffer (pH =3) and acetonitrile with 0.5mL/min flow in C-18 reverse phase column and 7 min of retention time. A diode array detector (DAD) at 275 nm was used for vitamin estimation. The method showed a good linear range of 0.01-10 µg/mL for analysis of B1, B3, B6 with LOD of 0.025 µg/mL and 0.1-10 µg/mL for vitamin C, with LOD of 0.1-10 µg/mL. The method validation parameters like precision, accuracy, linearity, limit of detection (LOD), RSD (%), and recovery (%) were studied. The result suggested that this method can be preferred for qualitative and quantitative estimation of vitamin B1, B3, B6 and C in green leafy vegetables and other sample matrices of the plant origin.

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Phenazine Functionalized “*opto-electronic nose*” for ammonia/aliphatic amines sensing @ Prostate Cancer Biomarker Sensor with Food Spoilage Evaluation

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Abstract:

Keeping in mind the urge of providing a single solution of multiple problems in real day scenario, multi-functional phenazine based dual-channel chromo-fluorogenic “*opto-electronic nose*”, **CN-2** has been synthesized in a single step *via* catalytic FeCl3 mediated facile oxidative C-N bond fusion of *o*-anisidine in neat condition with SC-XRD authentication. In-situ generated monoprotonated imine site made **CN-2** suitable for chromo-fluorogenic detection of ammonia/aliphatic amines (primary, secondary and even tertiary) over aromatic amines (ppm to ppb level) *via* target-specific deprotonation , well correlated with the outcome from Smartphone APP. Interestingly, aliphatic biogenic amines, like putrescine, spermidine detection capability made it a smart food-spoilage indicator and a potential prostate cancer biomarker sensor for clinical use as well, which alleviates the need of biopsies. One step ahead, fabrication of portable device using functionalized “smart” hydrogel assay with *all-in-one* **CN-2** escalates the reliability and practicability of present work through simple „*naked eye*‟ colorimetric-optical readouts.

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Using interfacial organic solvents in preparation and crystallization

~ Towards microfluid applications and safety of experiments ~

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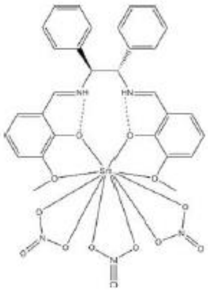
Abstract:

In our laboratory, organic solvents are used to prepare and form single crystals of rare earth complexes of Schiff base (Scheme 1) [1]. Since crystals are formed by volatilizing the organic solvent in solution, there is a risk of leakage. Indeed, the results of environmental measurement in our laboratory may potentially suggest both fire and health hazards [2]. When organic solvents volatilize to fill a room of laboratory, the vapor must be harmful to human health.

In this context, information, or knowledge of "interfacial organic solvents" used in preparation (two layers in test tubes) and crystallization (mutually dissolving solvents and solutes; vapor diffusion method) (Figure 1) will be important or useful for experimental design of microfluid preparation devices in near future. From the viewpoint of such analogy, in this presentation, we will present chemistry using interfacial organic solvents taken from our conventional experiments.



Scheme 1. Sm(III) complex.

Figure 1. Crystallization in tubes.

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Fixation of CO2 on multiple sites of the epoxides catalysed by a new microporous zinc phosphonate for isocyanate-free polyurethane synthesis

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Abstract:

Chemical fixation of CO2 on reactive organics species under mild reaction conditions is extremely difficult from the standpoint of sustainable fine chemical synthesis. Herein, we present the synthesis of a new microporous zinc phosphonate (ZnGLy) under hydrothermal reaction conditions employing *N*,*N*-bis(phosphonomethyl)glycine as a bridging phosphonate precursor. The high surface area of ZnGLy (108 m2/g) with regular microporous channels, as well as the presence of both Lewis acidic and basic sites, compelled us to investigate its catalytic potential for CO2 chemical fixation over a series of reactive organic compounds.1 ZnGLy exhibited excellent catalytic performance towards mono to tetra-cyclic carbonates synthesis with a broad substrate scope, including biologically active epoxides. Furthermore, the carbonates used as precursor for the model carbamate synthesis by the aminolysis reaction with the amines under solvent free reaction condition.2 By inspired from the model carbamate synthesis, the bis-cyclic carbonate derivative of bis-phenol A used for isocyanate-free poly(hydroxy)urethane synthesis.

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Pilot-scale Production of Sustainable Radiative Cooling & Fluorescent Material from Rice Straw

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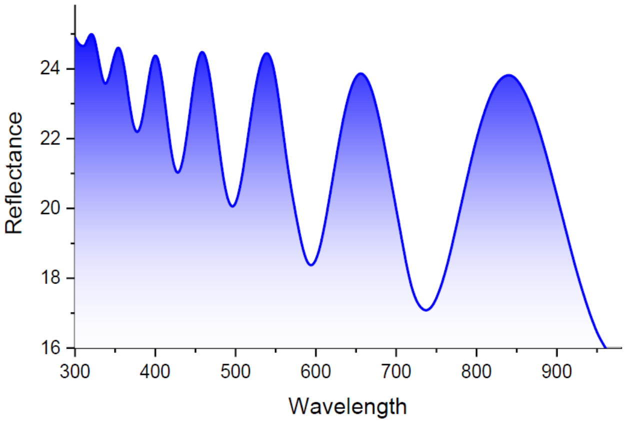
Abstract:

The agricultural waste generated in our country is mainly burnt on the field itself. And the burning of rice straws causes numerous health hazards, even choking metro city, Delhi. First, we have developed an economical method to separate microcrystalline cellulose (MCC) and lignin from rice-straw. This methodology can easily be translated to every-household of farmers. Moreover, we have demonstrated the use of MCC in making paper, sustainable fire-proof material and sedimentation filters. Our innovative strategy for production of value-added product from rice straw involves production of pure cellulose and lignin. We converted lignin into a fluorescent material by one-pot synthesis and transformed MCC into nanocellulose. Moreover, cellulose nanocrystal film can be used as a reflective cooler for energy-saving applications. In future, nanocellulose will be used for CO2 capture and extraction of Uranium from Seawater.



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SMART PROCESSING OF POLYMER PRODUCTS IN 3D MODE FOR SUSTAINABLE DEVELOPMENT

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Abstract:

Software mediated processing of solid polymers has emerged as a new, energy conducive smart technology within the last 10 years or so. In contrast to the conventional processing, the molten polymer is extruded on a temperature controlled open bed for solidification through crystallization following commands from computer aided manufacturing (CAM) software. The extruder head, commonly called the print head, extrudes the molten polymer filament first in XY direction, on completion then moves to Z direction to cover another XY layer and subsequently on replication forms or prints the entire product. Fused Deposition Modelling or FDM as the process is referred to, skips many tedious stages of product development in classical model e.g., numerous trials conducted for design, prototyping etc., costs of robust and expensive machine tools and molds and higher fixed head costs. Products made from crystalline thermoplastics, blends of plastics and rubbers, thermoplastic elastomers and polymer composites can be conveniently produced using this technique. Nevertheless, there are a few critical challenges subject to modus operandi e.g., rate of crystallization vs. crystallinity regain, rate of solidification of each printed layer vs. matrix coherency achieved at each printed layer, number of printed layers assigned to achieve the product thickness and the polymer infilling rate, are still needed to overcome before the process becomes fully scalable. This paper provides an overview of FDM processing side by side demonstrates non-traditional processing of a crystalline thermoplastic and its blends with an elastomer vis-à-vis their conventional processing for elucidation.

Keywords: 3D printing, Crystallinity, Rubber-Plastic Blend

Recent Advancement of Industrial Water Treatment Using Modified Polysaccharides

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Abstract:

Flocculation is a crucial event in the treatment of industrial wastewater. Because they are inexpensive and simple to use, inorganic coagulants (salts of multivalent metals) are widely employed. However, their limited flocculating ability and the existence of residual concentration of metals in the treated water limit their utilization. Due of their extraordinary capacity to flocculate effectively at low dosages, organic polymeric flocculants are now frequently employed. However, its use is connected to a lack of biodegradability and the dispersion of monomer residue in water, which could be hazardous to human health. However, due to their low flocculating effectiveness and short shelf lives, natural flocculants are required in high dosages. Thus, to create specially crafted grafted flocculants, synthetic materials are grafted onto the framework of natural polymers in order to combine the greatest qualities of both. Hyperbranched polymers on the other hand possesses greater degree of branching and its resemblance with that of dendrimers make it more effective. Due to higher branching and hence greater porosity, solubility in increases to a great extent which make them good candidate towards aqueous medium. The development of various flocculants that were being considered for the treatment of industrial wastewater is described in this work in general terms. They will also have their flocculation performance evaluated and the flocculation mechanism addressed. However, the future perspective of using hyperbranched polymers in the field of flocculation has been discussed extensively.

Continuous aqueous phase reforming of a synthetic wastewater with AuNPs catalysts for Biohydrogen production

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Abstract:

Aqueous phase reforming produces hydrogen from **biomass-derived oxygenated compounds** such as glycerol, sugars, and sugar alcohols. APR is unique in that reforming is done in the liquid phase. The process generates **Biohydrogen** without volatilizing water, which represents a major energy savings and therefore produces emission free Hydrogen. In the purpose of expanding applications in the field of production of Hydrogen with the help of Bio nanotechnology, the **Biosynthesis** of **Gold nanoparticles (AgNps)** by aqueous reforming of a synthetic compound (brewery wastewater) supported on **activated Carbon.** It is observed that AuNPs has the catalytic performance for degradation of pollutants at industrial level. The Cl- AuNPs are optimized by visible **UV Spectroscopy** with the **Surface plasmon Resonance (SPR)** and **Quantum Dots.** Therefore, Nanoparticles (MNPs) exhibit the excellent **catalytic degradation** and **decomposition** of the pollutants making the environment cleaner and sustainable. Gold nanoparticles have also been found to possess superior optoelectronic and catalytic properties. Aside from getting used as a store and symbol of wealth, research has in recent years shown that gold (Au) nanoparticles can find effective application in water treatment. The high absorption capacity of gold nanoparticles has been utilized in removing mercury from contaminated water. AuNPs have unique properties such as high surface area per volume ratios, ease of surface modification and high stability and biocompatibility. These properties lead to a magnificent removal capacity and high **selectivity** towards a variety of target species compared to those of the conventional adsorbents. Here, **deactivation** of the catalyst is avoided because Gold Nanoparticles have greater stability, resistivity and longevity that can harness the coking and **regeneration** process.

Keywords :- Aqueous phase reforming, Biohydrogen, biomass-derived oxygenated compounds, Biosynthesis, Gold nanoparticles (AgNps),activated Carbon, UV Spectroscopy, Surface plasmon Resonance (SPR) , Quantum Dots. Catalytic degradation ,decomposition, selectivity, deactivation, regeneration.

Dr. Poulomi Roy

Extracting Green Hydrogen as Clean Fuel from Seawater by Electrocatalytic Water Splitting

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Abstract:

Hydrogen production is one of the ultimate solutions to provide energy with zero emission.[1] Electrochemical water splitting producing clean H_2 is one of such effective ways, which often consumes fresh de-mineralized water. Water scarcity in India is another growing problem, which also need immediate solution as half of India's population is facing water stress. Thereby to meet the clean energy demand without disturbing the water problem further, use of seawater for electrocatalytic water splitting may provide the much-desired solution. However, the presence of chloride limits the use of seawater due to dominating chlorine evolution reaction (CER) over oxygen evolution reaction (OER), especially under high current region.[2] Indeed, the green hydrogen production by electrochemical water splitting involves the use of highly expensive RuO_2 or IrO_2 at anode and Pt as cathode, which makes the hydrogen production costlier. Furthermore, RuO_2 or IrO_2 can easily be attacked and thereby corroded due to chlorine or hypochlorite production, while seawater is used. To deal with such problem, careful selection of electrode materials is required. Thereby, rational design of noble metal free electrocatalysts for seawater splitting blocking the CER and allowing OER at anode is one of the most ambitious approaches to meet energy demand without wasting usable water.

The presentation will discuss about the rational designing electrocatalysts, modification of their intrinsic properties and various strategies to lead effective oxygen production at anode suppressing Cl_2 generation and producing green hydrogen at cathode during seawater splitting.

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[2] S Khatun, H Hirani and P Roy, Journal of Materials Chemistry A, 9, 2021, 74-86.

Keywords: Hydrogen, Electrocatalysis, Oxygen evolution reaction, Hydrogen evolution reaction, Seawater splitting.

Dr. Poulomi Roy is a Senior Scientist at CSIR – Central Mechanical Engineering Research Institute. Before joining CSIR – CMERI, she was working as an Assistant Professor at Birla Institute of Technology Mesra. Dr. Roy is a Fulbright Fellow under Fulbright-Nehru Academic and Professional Excellence Award 2016-17 and visited University of Wisconsin – Madison, USA. She has also been recognized amongst top 2% scientists world-wide in three consecutive years evaluated by Elsevier B.V. Dr. Roy obtained her PhD from Indian Institute of Technology Kharagpur, India in 2007. She spent 3 years at Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany as a postdoctoral research fellow. Her research interests comprise of the development of nanomaterials based electrocatalysts and various carbonaceous materials for their applications in energy conversion and storage devices, including photocatalysis, electrocatalysis, water splitting, dye-sensitized solar cells, supercapacitors etc.

Dr. Debkumar Bhowmick

Chiral Induced Spin Selective (CISS) Effect Towards Chiral Separation and Asymmetric Carbon Center generation

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Weizmann Institute of Science, Israel

Abstract:

Nature prefers chirality, whereas most biological systems consist of single chirality. Many processes in biological systems involve electron transfer (ET) through chiral environments. Enantiopure compounds synthesis or separation from their racemic mixture is highly essential. The relationship between chirality and magnetism is still not a clear subject. Recent studies have shown that the transmission of electrons through chiral systems is spin dependent. This phenomenon is known as chiral induced spin selectivity (CISS)[1,2].

Further, it is found that chiral molecules interact differently with spin-polarized paramagnetic substrates[3]. This phenomenon leads us to develop chiral separating systems by flow column or crystallization[4,5]. Similarly, the formation of a new chiral center in the presence of spin-polarized paramagnetic substrates can lead to enantioenhanced products. The spin polarization–induced chirogenic electropolymerization of achiral 2-vinylpyridine forms a layer of enantioenhanced isotactic polymer on the electrode[6]. The product formed is enantioenriched in asymmetric carbon polymer. This indicates that spin-polarized electrons can be used as an asymmetric catalyst.

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Dr. Deb Kumar Bhowmick working as postdoctoral research fellow at Weizmann Institute of Science. He obtained his Ph.D. at University of Muenster, Germany. He continued there as postdoctoral fellow another 2 years. Then, Dr. started second postdoctoral research at Chemical Physics department at Weizmann Institute of Science from 2019. His research work is centered at the interface surface science of organic, organometallics, biomolecular systems, material science, electropolymerization, enantioseperations. Currently, his is focused on the development of separating systems for enantiomeric compounds and electron spin induced enantiomeric synthesis. He has authored ~12 publications, one patent.

Awards& Honours:

- Fellow from Graduate School of Chemistry, Münster (GSCMS), Germany 2009-2012
- Council of Scientific and Industrial Research (CSIR) 2008

Dr. Gourisankar Roymahapatra

Li-doped aromatic heterocyclic (FAH) molecules as a promising hydrogen storage material

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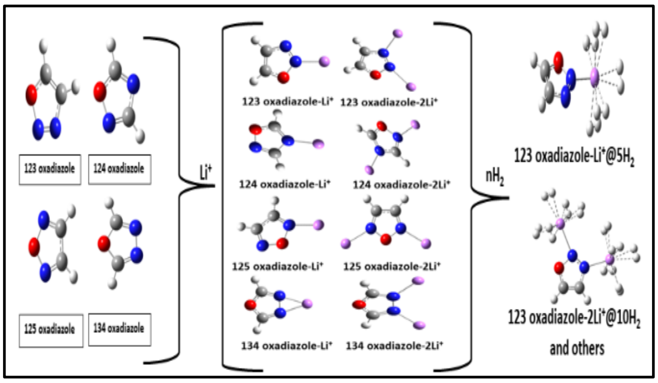
Keywords: Average adsorption Energy, Quasi-molecular Adsorption, Gravimetric wt %.

Abstract:

In search of potential hydrogen storage materials, we have taken aromatic heterocyclic (FAH) molecules (FAH = Imidazole, Pyrazole, Oxazole, Isooxazole, Thiazole, and Isothiazole, Oxadiazole isomers, Thiadiazole isomers). All FAH molecules can bond with both one and two lithium (Li) and we got maximum FAH-Li$^+$@5H_2 and FAH-2Li$^+$@10H_2 respectively with remarkable Gravimetric wt % with respect to minimum target set by U. S. Department of Energy. Again, FAH molecules have been identified as a promising hydrogen storage material since the average adsorption energy per H_2 molecule supports a quasi-molecular adsorption process.[1] According to the NBO analysis, the charge on the Li atom progressively drops with the gradual increase of H_2 adsorptions, indicating that a charge transfer interaction occurs between the bonding orbitals of H_2 molecules and the antibonding orbitals of Li.[2] According to the atoms in molecule (AIM) analysis, adsorbed H_2 interacts with Li through ionic type interactions.[2] Gibbs free energy change have been calculated to find out the spontaneous hydrogen adsorption temperature. The findings are very encouraging and exciting for synthetic chemists.

Scheme:



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2. M. K. Dash, S. Sinha, H. S. Das, G. C. De, S. Giri, **G. Roymahapatra**, *Sustainable Energy Technologies and Assessments*, **2022**, 52, 102235. doi: org/10.1016/J.SETA.2022.102235

3.

Dr. Gourisankar Roymahapatra, currently working as an Associate Professor of Chemistry at the School of Applied Science and Humanities in Haldia Institute of Technology, Haldia, West Bengal, India, is a passionate researcher of chemistry. He completed his Ph.D from Jadavpur University, Kolkata in the year 2014 with N-Heterocyclic Carbene Chemistry as a major field. Dr. Roymahapatra graduated (B.Sc) from Midnapur College under Vidyasagar University in 2000. He did his M.Sc in Physical Chemistry (2003) and M.Sc in Organic Chemistry (2005) from CSJM University, Kanpur, India. Before coming to academia, he worked as a Senior Chemist at MCC PTA India Pvt. Ltd, Haldia from 2003 to 2011. For his excellent contribution in quality control, he was awarded – 'Par Excellence in NCQC-2007' and 'Gold in CCQC -2010' by Quality Circle Forum of India (QCFI). In April 2011, he joined Global Institute of Science and Technology, Haldia, as a Lecturer in Chemistry and then he came to Haldia Institute of Technology, Haldia, on July 2015. He also worked as a Guest Lecture of Physical Chemistry at Midnapur College and Raja N.L. Khan Women's College, affiliated to Vidyasagar University, Student's counselor of Netaji Open University, Visiting professor of Haldia Institute of Management. His area of research interests includes - NHC complexes, Organometallics, Catalysis, Biological applications, Gas adsorption, Super alkali, Molecular modeling and DFT studies. For his contribution in research, he got 'Distinguished Young Scientist Award in Chemistry – 2014' and prestigious 'Bharat Gaurabh Award – 2018'. Dr. Roymahapatra is an elected Life Fellow of Institute of Chemists (India), FIC, and Life Fellow of Indian Chemical Society, FICS. He is the elected Vice-president of Haldia Vigyan Parishad from 2018-2020, and 2021-2023. His current research interest is on designing and developing new molecules and materials for hydrogen storage systems, and also to develop thin film semiconductors and super alkali materials for industrial applications. Dr. Roymahapatra is an editor of 'Education in Chemical Science and Technology', and 'Chemical Warta', published by the Indian Chemical Society and also the editorial board member and reviewer of several national and international journals.

Mr. Kamalendu Ghosh

RECENT TRENDS OF EFFECTIVE ENERGY UTILISATION TECHNOLOGY IN BISCUIT MANUFACTURING INDUSTRY

Kamalendu Ghosh
General Manager (Operations) & Head Of Technical-SOBISCO

Introduction:

In the present context of Indian scenario biscuit market particularly mass market has become very competitive in nature because of increasing trend of all cost component e.g., labour, power, fuel, ingredients & packing materials with price segment mainly Rs.5/- & 10/- in mass market variety/SKU & most common generic brand like Marie, Cracker, Glucose, Butter cookies & certain cream varieties. Reduction of pack weight also is very much limited as pack will look small & less customer appeal.

Labour cost is limited by Govt regulation & subject to automation.

Energy cost: It consists of power & fuel cost which is almost same for any unit with minimum required infrastructure & lot of scope is there to reduce energy cost substantially by utilising effective energy efficient technologies & some one time minimum investment. This will also help to reduce CO2 emission in environment.

Technologies of Reduction of power cost:

- Illumination: Minimum 400 lux is required for efficiency of man power & maintaining proper colour of the product. For this energy efficient LED tube light & bulb is recommend for reduction of illumination cost with better hygiene, proper colour of biscuit & man power efficiency.
- Variable Frequency drive(VFD) : In any Industry maximum power is used to run motors, Frequency drive is recommended for all the motors at least for more than 1hp motors, this will reduce power cost at by 15-20 % & life motor will be doubled because reduction of initial torque to minimum possible level. Frequency drive is also used to vary speed of machine as per requirement so better quality & quantity is ensured. Maximum power is consumed by mixers, sugar grinders, compressors, Oven circulating & turbulence motors & it is drastically reduced by VFD.
- **Energy integration in mixers** : Conventionally mixing /dough consistency is judged by mixing operator subjectively by hand feeling & eye observation, which varies from man to man & time to time for same man, this will not only impart inbuilt variability in process & product, also energy cost is increased as they increase mixing time with slow & fast RPM. This variability & energy cost can be reduced by utilising Energy integration technology in mixer. Depending on the Sedimentation value /Sedimentation index we need to fix Energy value for a variety/recipe/batch size e.g. 980KWH for one batch Marie with 290kg flour. Though fixing of energy for a particular batch of flour is done based on experience, but variation of energy & consistency of product for a particular batch is minimised.

I, **Kamalendu Ghosh** having academic back ground B.Tech (Food Technology & Biochemical Engg- 1989) & MBA (HR-2002-IBM) from Jadavpur University, completed 33 years of service in soft drinks & Biscuit Industry since 1989.

I have started my journey as a Quality Control Officer in a soft drinks industry (Mango Frooti) & then Joined Britannia Industries Limited & worked 22years since Dec'1989 to Aug'2011 in Production, Quality Control, Operations, new product development, Factory Administration, Training & development of Production & Quality Control team, Technical Trouble shooting across Eastern India as an officer, Manager, Factory Manager/Unit Head, corporate Manager.

Since Sept'2011, I have been working as General Manager (Operations) & Head of Technical in SOBISCO group with the responsibility of stabilisation of newly made unit, Factory administration, compliances of legal & Statutory rules, technical trouble shooting of different units of the group including Biscuit & Snack Food.

At present I am unit head of one 3500Tonns/pm capacity SOBICO biscuit plant, product development of all domestic & export brands, leading technical trouble shooting of different SOBISCO unit of WB,Bihar, Maharastra & also leading a team of 600 containers/year export from product development to USA & Canada consumers ,consists of 2 renowned brand namely SOBISK & famous Sunkist.

Throughout my journey I have achieved so many mile stones e.g., highest ever production in 2 Units of Eastern India in 2010, successfully stabilised DGF & Forced convection Indian hybrid Oven (New Era) for high count & low-density cracker Biscuit (460 count/kg, 40.5 square & 6mm thickness) first time in India (2014), approximately more than 15% baking fuel reduction in 3units by energy efficient Technical concept.

Three green field projects have been stabilised by me in 2007, 2011 & 2017. I am also a certified Lead Auditor of ISO 22000 FSMS by SAI Global (Mumbai) in Oct'2008 & have been bestowed with the Training of Trainer by R&D, BIL.

Mr. Shubhradip Guchhait

Preferential location of dopants in the amorphous phase of oriented Regioregular Poly(3-hexylthiophene-2,5-diyl) films helps reach high power factor towards organic thermoelectrics

Zhong Y.; Untilova V.; Muller D.; ***Guchait S****.; Kiefer C., Herrmann L., Zimmermann N., Brosset M., Heiser T. and Brinkmann M.**

Abstract:

Doping polymer semiconductors is a central topic in plastic electronics and especially in the design of novel thermoelectric materials. In this contribution, we demonstrate that doping of oriented semi-crystalline P3HT films with the dopant tris(4-bromophenyl)ammoniumyl hexachloroantimonate), also known as magic blue (MB), helps reach charge conductivities of up to 3000 S/cm and thermoelectric power factors (PF) of the order of 170±30 mW/mK2 along the polymer chain direction. A combination of transmission electron microscopy (TEM), polarized optical absorption spectroscopy and thermoelectric property measurements helps clarify the conditions necessary to achieve such high charge conductivities. The mechanism of doping is intimately related to the semi-crystalline structure of the polymer and whether crystalline, amorphous or both phases are doped. In the case of MB, mainly amorphous P3HT domains are doped while the structure of crystalline P3HT domains is almost unaltered by doping. A comparison with other dopants such as FeCl3, F4TCNQ, F6TCNNQ and Mo(tdf-COF3)3 indicates that the highest charge conductivities are obtained when the only amorphous phase of P3HT is preferentially doped. Charge transport improves in the sequence: i) doping of the only crystalline phase (F6TCNNQ and F4TCNQ), ii) doping of both crystalline and amorphous phases (FeCl3, Mo(tdf-COF3)3) and iii) doping of the only amorphous phase (Magic blue).

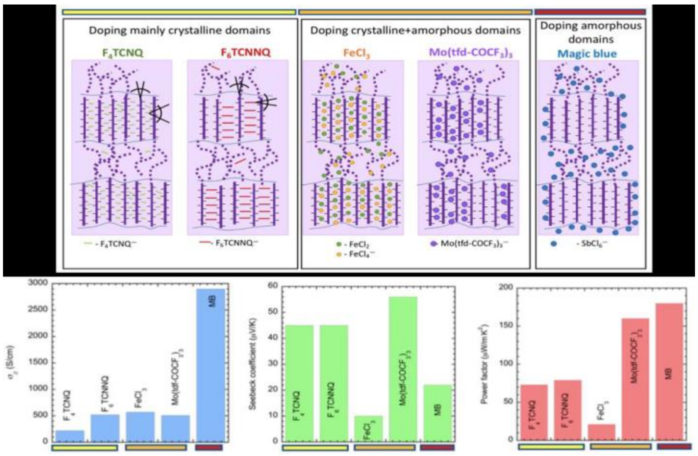

Figure 1: *Strategy of doping different regions of semicrystalline polymer correlates with maximum values of the charge conductivity, Seebeck coefficient and power factor measured in the polymer chain direction in oriented thin films of P3HT doped with different dopants.*

Shubhradip is a 2nd year PhD student working in Dr. Martin Brinkmann’s group in Institute Charles Sadron, CNRS, Strasbourg, France. He is an early-stage researcher in HORATES network funded by Marie Skłodowska-Curie Actions 2020. His thesis is mainly focused on orientation, structural control and doping mechanism of polymer semiconductor for thermoelectric applications. Before that he received his Master degree in Chemistry from Indian Institute of Technology Ropar and Bachelor degree in Chemistry from Ramakrishna Mission Vidyamandira (University of Calcutta).

Beside this, his constant motivation towards chemistry drove him to participate in several summer internships in some renowned institutes in India. In 2018, he worked with Prof. Sudip Malik in IACS Kolkata to prepare some smart electrochromic materials. In 2019, he worked with Dr. Supratim Banerjee in IISER Kolkata for the sensing of negatively charged biological analytes. In 2020, he worked with Dr. Pradip Kumar Tarafdar on Honeycomb-like structures on aqueous dispersion of honey, sugars and viscous liquids in IISER Kolkata. Also, he got an offer for three months summer internship from Prof. Arnaud Weck at University of Ottawa, Canada to work on electrochemical reduction of CO_2 in 2020.

Publications-

1) Y. Zhong, V. Untilova, D. Muller, **S. Guchait**, C. Kiefer, L. Herrmann, N. Zimmermann, M. Brosset, T. Heiser, M. Brinkmann, *Advanced Functional Materials* 2022, **32**, 2202075.

2) H. Zeng, P. Durand, **S. Guchait**, L. Herrmann, C. Kiefer, N. Leclerc, M. Brinkmann, *J. Mater. Chem. C*, 2022.

Dr. Santanab Giri

Heterocyclic Superhalogen: a potential molecule for the Li-ion battery electrolyte additive and activation of small molecule

Santanab Giri

School of Applied Science and Humanities, Haldia Institute of Technology, WB INDIA, 721657

Abstract:

Superhalogen is a special kind of molecule, which can not only mimic the properties of a halogen atom but also have more oxidising power. It has been observed that beside inorganic systems, organic aromatic systems are also behave like superhalogen. First principal calutaion on B-doped thiazole (C_3H_3NS) suggest its superhalogen behavior[1]. The superhalogen property can be further tuned, when three H atoms in bora-thiazole (C_2H_3BNS) have been substituted by more electron withdrawing groups like -F, -CN, -NO_2. The calculated EA and VDE of these systems i.e., (C_2F_3BNS), [$C_2(NO_2)_3BNS$], [$C_2(CN)_3BNS$] are higher than the halogen atom and can be consider as "Superhalogen". The potential applications of these molecules in Li-ion electrolytes/ additives and activation of small molecules like H_2, H_2O have been exploed in this work. We could able to show that our designed superhalogen [$C_2(NO_2)_3BNS$] can be used as Li-ion battery electrolyte[2]. Not only that, they have potential to act as an additive also[3]. These heterocyclic Superhalogens can act as a building block of Lewis acid which can make frustrated Lewis pair (FLP)[5, 6] with a well-known Lewis base i.e., P(tBu)$_3$. Further, these FLPs can activate the small molecules (H_2, H_2O) more efficiently than the traditional FLP.

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Dr. Santanab Giri is currently working as an associate professor in the School of Applied Science and Humanities, Haldia Institute of Technology. He received his BSc (Chemistry Honors) and MSc (Chemistry) degrees from Vidyasagar University, West Bengal. After that he joined the research group of Professor P. K. Chattaraj for his PhD degree in the Department of Chemistry, Indian Institute of Technology, Kharagpur as an Institute Fellow. In 2011, he moved to Pontificia Universidad Catolica de Chile for his postdoctoral study with Professor Alejandro Toro-Labbe. After finishing his first postdoctoral tenure, he moved to Virginia Commonwealth University, USA in 2013 to work with Professor Puru Jena. Dr. Giri returned to India as a DST Inspire Faculty. He worked in this position in NIT Warangal and NIT Rourkela from 2014-2018. For the last 10 years, he is actively involved in designing metal clusters, molecules with unusual properties using density functional theory and abinitio molecular dynamics techniques. He has more than 150 journals of International repiute and 10 book chapters. He has successfully carried out several projects funded by Govt. of India. He is also a recipient of two national awards (Professor Santi Ranjan Palit award and Sir P. C. Ray award) and one international award (Eli-Lilly Asia Outstanding Thesis Award). Dr. Giri is a ‘Life Fellow of the Indian Chemical Society, Chemical Research Society of India, Indian Photo-biology Society and Orissa Chemical Society.

Dr. Soumendra Darbar

Sanative Effect of Surface Functionalized Mn_3O_4 Nanoparticles upon Chronic Hepatic Dysfunction in Experimental animals

Soumendra Darbar[1,2], Srimoyee Saha[2] and Atiskumar Chattopadhyay[2]

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[2]Faculty Council of Science, Jadavpur University, Raja S C Mallick Road, Kolkata-700032, India

Abstract

Currently, there is a great deal of interest in the health benefits of inorganic NPs. In the past two decades, several NP-based therapeutics have been successfully introduced for the treatment of cancer, pain and infectious diseases. However, uses of inorganic NPs in treatment of chronic diseases are sparse in literature. Chronic liver diseases are the fifth most common cause of death, affecting around 400 million people per year worldwide and have no effective medication. The aim of this study was to evaluate potential hepatoprotective activity of orally administered citrate functionalized Mn_3O_4 nanoparticles (C-Mn_3O_4 NPs) against CCl_4 induced hepatotoxicity. Our results show that oral treatment of C-Mn_3O_4 NPs can effectively reduce severe chronic liver damage even fibrosis in CCl_4 -induced mice model. Further investigations revealed that C-Mn_3O_4 NPs show increased antioxidant activity upon acid treatment (both in vitro and in vivo i.e., stomach), which is in turn responsible for its hepatoprotective nature.

Assessment of various liver function parameters along with histopathology and immunohistochemistry were performed to evaluate pathophysiological condition of the liver. To unravel the mechanisms involved in attenuation of liver injury by NPs, various antioxidant parameters (like superoxide dismutase, catalase, glutathione peroxidase, reduced glutathione etc.) were also examined. An in depth study of the effect of C-Mn_3O_4 NPs on mitochondria, the cellular mediator of oxidative stress further revealed the molecular mechanism behind its therapeutic efficacy. To best of our knowledge, this is the first study that demonstrates direct oral treatment of an inorganic NPs (i.e., C-Mn_3O_4 NPs) without any delivery system can efficiently reduce chronic hepatotoxicity and liver fibrosis through its antioxidant activity

Dr. Subrata Ghosh

Near Infrared Emissive Optical Markers for Albumin: A Platform for Bioimaging

Subrata Ghosh
School of Chemical Sciences
Indian Institute of Technology Mandi

Near infrared region (NIR) constitutes a significant part of the electromagnetic spectrum ranging from 700-1700 nm. NIR region can further be divided into NIR-I window from 700-900 nm whereas NIR-II lies beyond 1000 nm and continues until 1700 nm. Besides the several usefulness of this region, in biomedicine it has significant relevance. NIR region possess advantages over the visible region owing to the higher tissue penetration depth, minimized autofluorescence from biomolecules and reduced photon scattering resulting into images with high contrast and higher resolution. On moving from NIR-I to NIR-II region, the absorption and scattering is further diminished resulting into superior imaging quality. Although, a lot of efforts have been directed towards development of NIR probes, however, only two of these (Indocyanine green and Methylene blue) could be approved by FDA for further application in the clinics. Literature demonstrates the significance of these FDA approved dyes in potential biomedical applications such as in diagnosis and monitoring diseases, guiding surgical interventions and evaluate treatment efficacy and prognosis. ICG have found widespread uses in hepatic, cardiac, and ophthalmologic studies, and is being used for analysing tissue perfusion and identification of sentinel lymph nodes in cancer staging.

Attributed to such critical usefulness of the NIR-I dyes, attempts have been now directed towards development of suitable NIR-II emissive materials owing to the superior imaging ability over NIR-I region. Small molecular probes in this aspect have inherent advantage over other inorganic and nanomaterials owing to their smaller size which is far below the renal cut-off size (~5 nm) and molecular mass (< 40 kDa), making them suitable contrast agents for clinical translation. Despite the tremendous efforts, albumin specific NIR-II emissive optical markers are rare. Considering this, the recent developments towards serum albumin specific molecular markers emitting in NIR-I developed by our lab will be highlighted in this talk following brief discussion on their design strategy. The crucial significance of albumin in the human body and its importance as a biomarker for various diseases will be elaborated. Furthermore, the modulations in the serum albumin levels under various pathophysiological states through successful visualization utilizing the developed probes will be emphasised here.

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Subrata Ghosh completed his master studies at Visva-Bharati University and doctoral studies at the Department of Chemistry, IIT Mandi under the supervision of Prof. A. T. Khan. He then moved for postdoctoral studies at three different places – Bar-Ilan University, Israel; Case Western University, USA and University of Leipzig, Germany. He joined IIT Mandi in 2010 and has been the serving the same Institute since then. His research interests include organic synthesis and organic materials for practical applications.

Dr. Debdas Roy

How to harvest organic triplet energy at ambient conditions?

*Nirmalya Achrya, Suvendu Dey, Manoj Upadhyay, Raktim Deka, Debdas Ray**
Department of Chemistry, Shiv Nadar Institution of Eminence, Deemed to be University,
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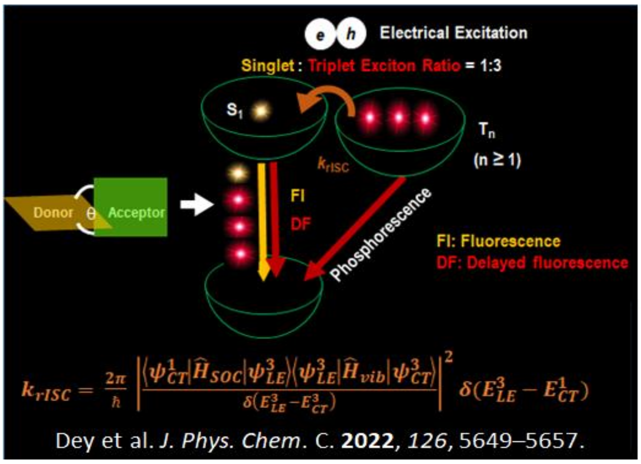
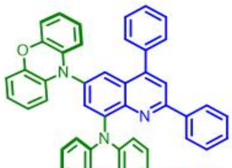
Abstract:
Borrowing an idea of delayed fluorescence, Perin (1929)[1], Lewis (1941)[2], Parkar (1961) and Hatchard (1968) in the two papers[3,4] proposed the idea of E-type delayed fluorescence in Eosin and Benzyl. This emission mechanism, now known as thermally activated delayed fluorescence (TADF) was recently reinvigorated by Adachi and others, who proposed it as a way to harvest non-emissive triplet excited states in organic light emitting diodes (OLEDs).[5] The TADF occurs via reverse intersystem crossing (RISC) from the lowest triplet to the singlet state mediated by vibronic coupling between triplet manifolds (**Figure**). The RISC mechanism is a key ingredient of the triplet energy harvesting in chemical physics for generating 100% internal quantum efficiency. In this presentation, an overview of the search for and the discovery of the organic triplet, the subsequent measurements of the properties of the new organic systems, and the future directions in this area of research will be addressed by the speaker.[6]



$$k_{rISC} = \frac{2\pi}{\hbar}\left|\frac{\langle\psi^1_{CT}|\hat{H}_{SOC}|\psi^3_{LE}\rangle\langle\psi^3_{LE}|\hat{H}_{vib}|\psi^3_{CT}\rangle}{\delta(E^3_{LE}-E^3_{CT})}\right|^2 \delta(E^3_{LE}-E^1_{CT})$$

Dey et al. *J. Phys. Chem. C.* **2022**, *126*, 5649–5657.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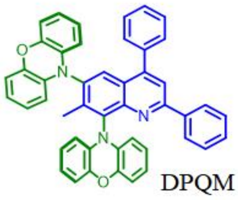
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Debdas Ray, associate professor of the Department of Chemistry, Shiv Nadar University, Delhi-NCR, has earned his Ph. D. degree (PI: Professor Parimal Kanti Bharadwaj) from Indian Institute of Technology Kanpur. His doctoral research work was based on the selective detection of biologically important metal ions using fluorescence signaling. He had also explored other research scopes outside India (France, USA, Japan), and significantly contributed to the groups. Presently, Dr. Ray is having more than ten years of experience in photophysics and photochemistry background. He has successfully applied various spectroscopic techniques to study and understand the excited state dynamics of molecular systems for triplet energy harvesting for OLEDs, data security, photosensitizer, and sensors. In India, he has developed a new research area of triplet energy harvesting via up-conversion of excited triplet state to singlet (i.e., thermally activated delayed fluorescence) state along with persistent-emission at ambient conditions.

His research outcomes have been published in highly reputed journals, and cited by high impact journals. Recently, he has invented “invisible ink” which had published in thirty-four national and international newspapers. Recently, he has published two ACS articles (J. Phys. Chem. Lett.) in single volume, which is one of the rare achievements of his research activity (highlighted by ACS-live slide presentation). Furthermore, he has successfully developed a novel and un-explored route to allow efficient harvesting of triplet energy above RT.

Dr. Atis Kumar Chattopadhyay

Green Synthesis of a Nano-conjugate and its application in Drug Development

Atiskumar Chattopadhyay

Faculty of Science, Jadavpur University, Kolkata-700032, India

Nanomedicine is becoming a promising weapon to treat various communicable and non-communicable diseases.The target specificity of nano-conjugates is being used for prevention and treatment of diseases.Liver fibrosis, a reversible pathological process of inflammation and fiber deposition caused by chronic liver injury can cause severe health complications, including liver failure, liver cirrhosis, and liver cancer. Traditional drug-based therapy has several limitations, such as lack of precision and inadequate therapeutic efficiency. As a medical application of nanotechnology, nanomedicine exhibits great potential for liver fibrosis diagnosis and therapy.We developed a novel nano-conjugate coupled with Andrographis paniculata (AP-Ag NP), through green synthesis, acted as a nanozyme in mammalian system. For development of Oxidative stress and inflammation one group of mice were exposed to carbon tetrachloride (CCl_4) for 8 weeks and another group co-administered orally with AP-Ag NP (50 mg/kg each) to evaluate redox scavenging activity. The results suggest a significantly elevated ROS, decreased blood and hepatic GSH levels, superoxide dismutase and catalase activities after carbon tetrachloride (CCl_4) exposure. Co-administration of (AP-Ag NP) increased SOD, CAT and GSH levels and was also beneficial in the recovery of oxidative injury and restoring inhibited aminolevulinate dehydratase (ALAD) activity. Our results suggest that AgNP synthesized using Andrographis paniculate (AP-Ag NP) have the potential antioxidant activity in experimental animals, which can be applied for future drug development. .

Keywards: Silver Nanoparticle, Green Synthesis, Liver Fibrosis, Oxidative Stress, Antioxidant

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EDUCATION:

1. **B.Sc. (Honours) in Physiology**, with Physics and Chemistry as subsidiary subjects, **Presidency College, Calcutta,** (*1985, Examination held in 1986).*
2. **M.Sc. in Physiology**, University of Calcutta, *(1987, Examination held in 1988).*
3. **M. Phil in Environmental Science**, University of Calcutta *(1989, Examination held in 1991).*
4. **M. Tech. in Biotechnology,** Jadavpur University *(1998 – 2000).*
5. **Ph.D. awarded on 26.11.2015**. The title of the thesis is **"Studies on the effects of benzodiazepine derivative alprazolam on different tissues of rat"**, Jadavpur University.

AWARDS AND ACHIEVEMENTS:

1. **Invited Talk award** for the talk on **"Effects of Stress on Immune Regulation"** in the "6th International Science Conference" of World **Science congress** held at PGIMER, Dr. R.M.L. Hospital, new Delhi, on 23rd to 25th December, 2016.
2. **Editorial Board Member of** the journal ***International Journal of Pharmacy and Chemistry***.
3. **Reviewer of** the journal***Drug and Alcohol Dependence*** of Elsevier Publication.
4. **Reviewer of** the journal ***Biomed Research International***ofHindwai Publication.

Dr. Sanjib Das

Porous Organic Polymers: Diversity from Simplicity

Dr Sanjib Das, Principal Scientist,
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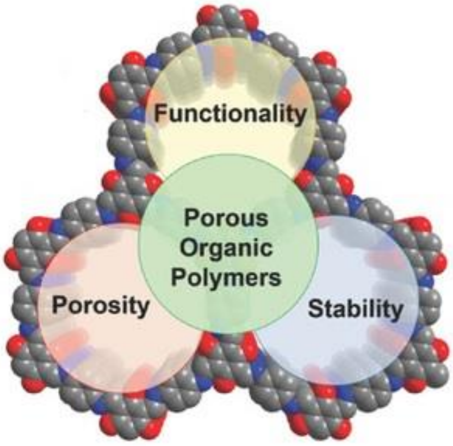
Porous Organic Polymers (POPs) are a class of multi-dimensional porous network materials, which are built via strong covalent linkages between various organic building blocks with different geometries, topologies and functionalities. Owning to their advantages of light-weight, superior inherent porosity, excellent stability, pre-designable and tuneable structures and functions, POPs have received increasing attention and research interest for their tremendous potential applications in various domains of materials science. Their porous structure, pore size, specific surface areas and functions can be directly designed and facilely tuned by introducing specific functional building blocks. In present talk, we summarize the latest advances in the field of POPs, focusing on their design, synthetic strategies and functionalities including ongoing research at CSIR-IMMT.



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Dr. Sanjib Das, currently working as an Principal Scientist in the Materials Chemistry Department at CSIR-Institute of Minerals and Materials Technology (IMMT), Bhubaneswar, Odisha, India. He completed his M.Sc in Chemistry (2000) from Banaras Hindu University, India and subsequently did his Ph.D in Chemistry from IIT Kanpur in the year 2007 under Prof. P. K. Bharadwaj. He then moved for postdoctoral studies at four different places – University of Hohenheim (2007), Germany; University of Heidelberg (2008), Germany; National Institute for Materials Science (NIMS), Japan Weizmann Institute of Science, Israel. He was also a visiting professor at Institute of Chemical Technology-Indian Oil Corporation (ICT-IOC), Bhubaneswar, India.

Selected Publications:

(1) Das, M.; Sarkar, S. K.; Patra, Y. S.; Manna, A.; Mukherjee, S.; Das, S., ACS Appl. Nano Mater. 2022, 5, 8783-8793.

(2) Manna, A.; Maharana, A. K.; Rambabu, G.; Nayak, S.; Basu, S.; Das, S., ACS Appl. Polym. Mater. 2021, 3, 5527-5535.

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Dr. Ashok Kr Jha

Bioremediation trends on mitigation of As(III) and Cr(VI) from aqueous medium using bacterial isolates and plant biomass

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Abstract:

Arsenic and chromium are the potential carcinogenic agents affecting a wider area in the world including Gangetic plain of India. Though several traditional methods are available, efforts have been made to use plant biomass and bacterial isolates for decontamination in view of plant abundance, technical applicability and cost-effectiveness. Bixa Orellana has been established as an accumulator of As (III) and Cr (VI) validated by SEM-EDX, FTIR and kinetic studies. The maximum percentage removal of Cr(VI) by B. Orellana is 82.8 for an initial concentration of 3 ppm. The R^2 values from experimental data best fitted to Freundlich as well as Elovich isotherm. The bacterial isolates from Rajmahal coal mines have showed As(III) resistance up to 150 ppm. The 16S RNA genotyping confirmed the similarity of these isolates with Stenotrophomonas maltophilia and bacterium E_1 The genes e.g aox, acr and ars were involved in arsenic biotransformation. The maximum percentage removal in 50 ppm initial concentration with ASBBRJM16 and ASBBRJM87 bacteria were 60.66 and 10.30 respectively. Thus, bacterial isolates may be adopted as an effective and eco-friendly alternative for removal of As (III) and Cr (VI) from aqueous medium

Keywords: - Biosorption, Bacterial isolates, Elovich Isotherm, Biotransformation, Genotyping

Dr. Ashok Kumar Jha is working in University Department of Chemistry, T. M. Bhagalpur University, Bhagalpur, Bihar. Dr. Jha has a brilliant academic career. He always stood first in merit and has been awarded National merit scholarship throughout. He has organized fifteen national, one international seminar and five webinars approved by U.G.C New Delhi, C.S.I.R. New Delhi, B.C.S.T. Bihar, NABARD and other agencies. He has delivered many invited talks in India and abroad. Dr. Jha has teaching and research experience of 36 years. His interest is reflected through his paper in different National and International journals. He has nine books to his credit. He has completed two research projects sponsored by UGC and has been working on the problem of arsenic and heavy metal contamination and their removal. He teaches solid state chemistry and quantum chemistry in post graduate course. He has more than 50 research articles in different National and International journals related to kinetics, co-ordination and adsorption of arsenic and heavy metals. Dr. Jha is the member of several academic societies and member of editorial team of many journals. He publishes a biannual journal “Jalchintan”.

Dr. Vijayakrishna Kari

Imidazolium based Chiral Poly(Ionic liquids): Synthesis and their Morphological Study

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Abstract:

Stereoregular helical polymers have attracted significant attention due to their wide range of applications in various fields that includes chiral organocatalysis and chiral resolution.[1,2] The helical morphology of the chiral polymers depends on the synthetic approach.

In our research group we have synthesized various responsive chiral poly(ionic liquids) (CPILs) and were successfully used in chiral induction with targeted chiral switch.[3-5] Here, chiral groups were linked to polymer via covalent and/or ionic means.[6] These CPILs are responsive polymers, whose conformation can be stimulated. A systematic study on the helical morphology of the synthesized chiral polymers were carried out and the same will be discussed in the presentation.

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Vijaykrishna Kari, Associate Professor of the School of Basic Sciences, IIT Bhubaneswar, Odisha, has earned his Ph. D. degree from Indian Institute of Technology Madras. He subsequently did his postdoctoral research experiences from LCPO, University of Bordeaux-1, France as CNRS Postdoctoral fellow. His research interests is in synthesis of chiral polymers, MIPs, resins and PILs for the application of gas separation membranes, nuclear waste treatment and drug delivery system. He was also a visiting scientist at University of Basque countries, Donostia-San Sebastian, Spain & ITQB, Lisbon, Portugal from May 2016–July 2016 and then Universidad del País Vasco/Euskal Herriko Unibertsitatea (UPV-EHU), Donostia-San Sebastian, Spain (Nov 2013–April 2014). He has guided 6 doctoral students and published more than 75 journal articles and 3 patents.

One-pot green synthesis of nanoparticles and its various applications

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Abstract:

The term nanoparticle is used to describe a particle with size in the range of 1–100 nm at least in one dimension. There are numerous methods for synthesis of nanoparticles, such as physical, chemical and biological but, biological method is mostly used. Many previous researchers highlighted the green synthesis of heavy metal nanoparticles. Green synthesis of nanoparticles has some advantages towards the reduction of metal ions and their stability. Nowadays, there is a wide application of nanoparticles in diverse fields including catalysis, energy, optoelectronics and medicine. Nanotechnology approaches to control disease in human and plants have recently been increasing greatly and the unique physicochemical properties of nano-sized metal particles make them successful in biology and medicine. Particularly, in this discussion, some specific areas where nanoparticles can be applied to overcome the environmental problems. One such major problem is mosquito population. Mosquito-borne disease represents a deadly threat to millions of people worldwide. They transmit various disease like, west Nile fever, malaria, dengue, chikungunya, zika, and filarial. Many chemicals like dichlorodiphenyltrichloroethane, dieldrin, organophosphorus, fenitrothion, and many physical processes like a light trap, mosquito net, electric net and many phytochemicals are commercially used for controlling mosquito. Till today, researcher can't reach their satisfaction level for controlling this insect. National vector born control disease program, India's report suggested that till now mosquito is a big threat throughout the India. . From this background, present discussion will highlight to synthesis botanical one-pot synthesis of nanoparticles and their judicial application towards control of mosquito population.

Keywords: Plant parts; metal nanoparticles; Green synthesis; Biomolecules; Mosquito population

Dr Naba Kumar Mondal is currently holds the position of Professor in Environmental Science, Department of Environmental Science, The University of Burdwan, Burdwan, India. He completed his post graduate in Chemistry from the Department of Chemistry and doctorate degree in Environmental Science from Department of Environmental Science, The University of Burdwan. Prof. Mondal established a resourceful high quality Environmental Chemistry laboratory in the Department having quality research instruments. He has published his research work more than 300 (Total citation: >4400) reputed International and National journals and a recent book entitled "Intelligent Environmental Data Monitoring for Pollution Management" as co-Editors. Since date he guided 17 Ph.D. among them 16 have been awarded and one submitted and currently four Ph.D. students and one D. S. Kothari pdf scholar also working under prof. Mondal. Moreover, he also guided more than 65 M.Sc. theses and 2 M.Phil. fellows. Since today he had 11 research projects in his name as a Principal and/or Co-PI which amounts more than 1.70 crore from various funding agencies like DST-GoI, UGC, WB-DST, ICAR, ICSSR, BRNS etc. His primary research interest are Adsorption Chemistry by low cost adsorbents, Water quality degradation and management in Arsenic and Fluoride affected areas of West Bengal, Indoor Air Pollution and Human Health, Nanotechnology and Mosquito control, Mobile tower radiation and Human health, and Teacher Education. Prof. Mondal has delivered several invited talks and key note addresses in National and International conferences of high repute. He had chaired various International and National seminar and conferences. He served as coordinator of UGC sponsored various refreshers courses and also secretary member of WB-DST sponsored Science Congress. Prof. Mondal also served Editorial Board member, Editorial advisory committee member, etc. of various journals as: International Journal of Applied Nanotechnology, Archives of Environmental Sciences and Environmental Toxicology, Biochemistry and Analytical Biochemistry, The Global Environmental Engineers, Journal of Environmental Science and Social Sciences, etc.

Prof. Mondal has been nominated as reviewer of reputed publication houses like Elsevier, Springer's, Taylor and Francis etc.

Recently, Prof. Mondal was enlisted in world 2% scientist as published by Stanford University

Preparation of three-dimensional metal-organic-framework for the fluoride chemisorption and photodegradation of carcinogenic dyes

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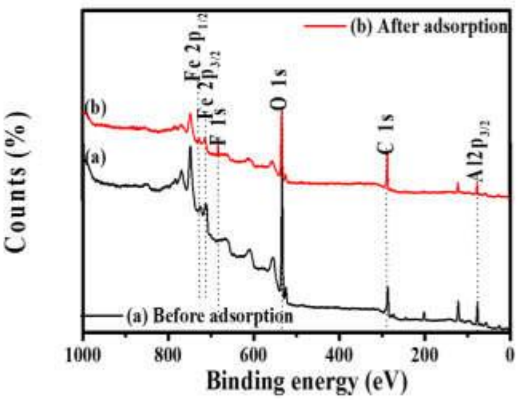
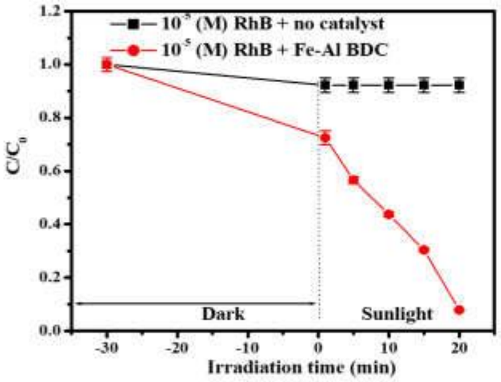
Abstract:

In the modern era water pollution is a serious issue. Fluoride contamination into water bodies is a natural and anthropogenic reason. The growing textile industries release toxic colored wastewater into the waterbodies without proper treatment. A 3D rod-like, porous Fe-Al bimetallic metal-organic-framework (MOF) with 1,4-benzenedicaboxylic acid as an organic linker (abbreviated as Fe-Al BDC) was prepared using the solvothermal method for the fluoride chemisorption and photodegradation of toxic dyes. Fe-Al BDC with 120.255 m2/g surface area was able to remove fluoride 95.60 % within 45 min from 10 ppm initial fluoride solution at pH 7. The chemisorption of fluoride was confirmed from the FTIR and XPS studies. Fe-Al BDC was used for the photodegradation of carcinogenic water-soluble xanthene dye rhodamine B (RhB) (10-5/10-4 M) (pH range 2-11) under the Solar irradiation. The photodegradation mechanism was established using HPLC and LC-MS studies. The Fe-Al BDC MOF was reusable up to eight cycles.





Magnetized Water as a Bio stimulant for High-Yielding Crops, Fragaria x Ananassa: *Experimental Insights from Structural Design, Finite Element Method Simulations, and Water Molecule Microstructure Analysis*

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Abstract:

The purpose of this investigation was to better comprehend the mechanisms and instrumentation of fluid (i.e., water) magnetization, in addition to its application and experimental findings on recent advancements to its applicability and novel green technology, in particular for typical water-demanding plants that are heavily used during fruit-bearing seasons. High-yielding corpus strawberries have been shown to be the most effective physical growth stimulant, according to both established and newly published research. These strawberries have indeed been discovered to have profound effects on root function, plant chemical composition, and nutrient availability in the soil when exposed to magnetized water. Since it has the potential to be a bio stimulant and to have effects on human health and the environment, magnetized water necessitates a more thorough understanding of fluid magnetization dynamics, its relationship to the molecular structure of water, and instrumentation design.

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Tetracycline antibiotics degradation in an aqueous medium using ammonium phosphomolybdate as an oxidant

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Abstract:

Tetracyclines (TCs) constitute a group of broad-spectrum antibiotic drugs with varieties of applications. The release of TC residues into the surroundings and the inadequate elimination from the traditional treatment techniques result in their frequent occurrence over the entire environment. Ammonium phosphomolybdate (APM) serves as an effective oxidant for the degradation of TCs under ambient conditions. About 98% degradation of TC at a concentration of 20 mg/L is achieved through 90 min of reaction at pH ~ 4 using APM at a dose of 0.75 g/L. A possible reaction mechanism is proposed. The APM is recycled seven times with a TC degradation efficiency of 72.1%.

Recovery of Hydrogen and Sulphur by Electrolysis of H_2S

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Abstract:

The electrocatalytic decomposition of the abundant and toxic H_2S from industrial by-products is a promising energy conversion technology for H_2 production and for environmental safety.[1] But due to the lack of low-cost and efficient electrocatalysts, this technology for H_2 production is not being explored much. Herein, we have designed an efficient catalyst i.e., cobalt-doped CdS nanoparticles as the anode for highly efficient electrocatalytic H_2 production from H_2S. This optimized catalyst could drive the anode reaction at an onset potential of 0.25 V vs RHE which was 1.33 V lower than that required for the water oxidation reaction. The proposed catalyst was highly stable up to the 1000 cycles for sulfur oxidation reaction (SOR). Further, the solution of polysulfides obtained after H_2S electrolysis was treated with acid to obtain the powder sulfur. This recovered sulfur can be used as an electrode material for sulfur-based batteries.[2] Thus, this method demonstrates its great potential for hydrogen production and sulfur towards sustainable energy applications.

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Catalytic depolymerisation of polyester textile wastes using nanocomposites of g-C_3N_4 and doped ZnO

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Abstract:

PET, often referred to as polyethylene terephthalate, is a versatile commodity material that is frequently used in the manufacture of synthetic textile yarn and beverage bottles. Due to overexploitation of PET material, the management of PET wastes is become a global environmental issue. Chemical recycling is proven to be most successful process of PET waste recycling than physical recycling. The present research work aims to depolymerise PET waste from 100% pure polyester (PES) coloured threads as a model reaction for recycling PES textile wastes catalysed by g-C_3N_4 doped with bimetallic ZnO as a visible light photocatalyst. In our investigation, pure (P-g-C_3N_4) is mixed with 10wt% of metal-metal oxide (Sn0.02Zn0.98O) using wet-impregnation method. The nanocomposite catalyst characterised using XRD, FT-IR, UV-Visible, and surface morphology and elemental composition obtained from SEM-EDX. For the depolymerisation of PES coloured threads, aminolysis using Ethanolamine (EA) and glycolysis for Ethylene glycol (EG) to carry out the reaction to produce bis(2-hydroxy ethylene)terephthalamide (BHETA) and glycolytic product is bis(2-hydroxy ethyl)terephthalate(BHET) respectively. The depolymerised product were characterized for FT-IR, ^{13}C NMR, ^{1}H NMR, MS and the formation of BHETA and BHET.

Modified starch based selective flocculant for the beneficiation of low-quality iron ore: experimental and theoretical studies

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Abstract:

A selective flocculant, St-Meth-Co-PAM has been synthesized by functionalization of starch (St). Starch methacrylate (St-Meth) has been first developed by methacrylation of the starch with methacrylic anhydride (MAh) followed by formation of a 3D network like structure which has been achieved by free radical polymerization among St-Meth molecules and then grafting simultaneously with polyacrylamide chain on the St-Meth network backbone [1]. The developed selective flocculant has been characterized by several characterization techniques. The selective flocculation efficacy of the synthesized selective flocculant has been studied and compared with the industrial selective flocculant starch [2]. It has been established from the selective flocculation study that the material exhibit very good selective flocculation efficiency by means of settling velocity and iron recovery. Also, from the theoretical analysis, it can be said that the material form coordination with the hematite particles selectively [3]. That's why the material St-Meth-Co-PAM can be affordably used for industrial purpose as displayed very high settling speed and high iron recovery rather than the conventional selective flocculant starch.

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Chemical recycling of polyester textile wastes through Lewis acidic bimetallic ZnO nanocatalysts

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Abstract:

The current study focuses on the catalytic depolymerisation utilized in the recycling of polyester (PES) textile waste. By using the catalytic technique, PES depolymerised to generate bis(2-hydroxy ethyl)terephthalamide (BHETA) and bis(2-hydroxyl ethyl)terephthalate (BHET) under glycolysis and aminolysis reaction. As a recoverable nanocatalyst, biometallic zinc oxide nanoparticles doped with In, Cd and Sb were synthesised using the sol-gel technique at various 0.5, 1.0, 2.0 and 3.0 mol% of dopants. The crystallite size, surface morphology and composition of biometallic ZnO NPs were investigated using XRD and SEM-EDX. The modification in optical bandgap upon doping analysed using UV-Vis spectroscopy and Tauc's plot. All the bimetallic ZnO samples exhibit crystalline behaviour and a hexagonal wurtzite structure, with an average crystal size of 35 to 60 nm, according to the powder XRD pattern. The optical band gap of doped ZnO NPs was found to be between 3.21 and 3.19 eV, which is smaller than the band gap of pure ZnO NPs of 3.31 eV. Depolymerisation of PES textile wastes carried out using ethylene glycol and 2-aminoethanol under conventional and microwave heating. The catalytic efficiency of doped ZnO evaluated using catalyst:PET ratio, PET:reagent ratio. The aminolytic depolymerisation of PES offered higher conversion and yield of BHETA than glycolysis. The depolymerised products 1H and 13C NMR, FT-IR, and mass spectroscopy were used to describe the yields achieved (MS).

Resourceful utilization of methylene blue contaminated water for fabrication of ultra-stable supercapacitor device

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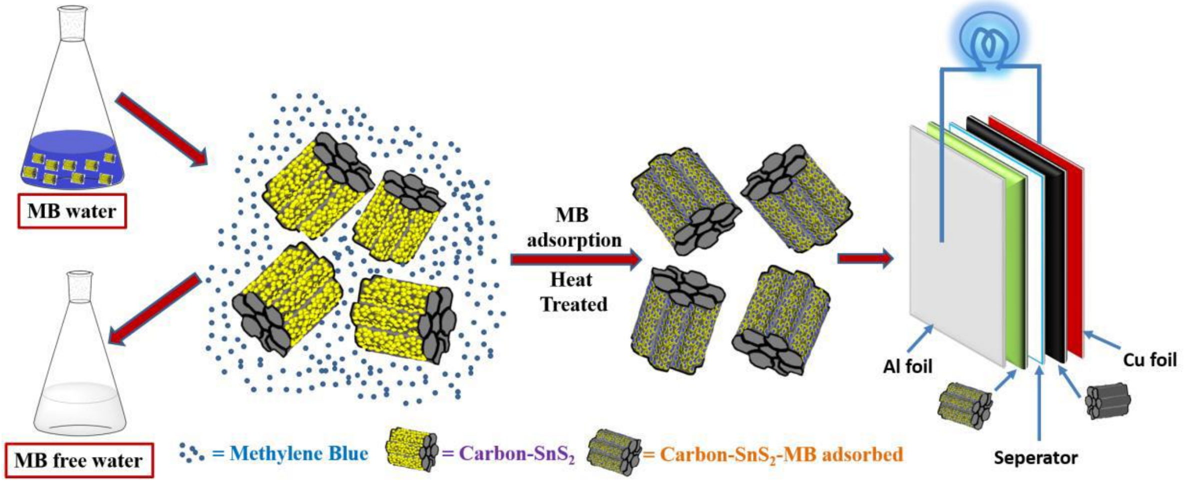
Abstract:

Carbon was synthesized through the carbonization of waste grass and was converted to Carbon-SnS2 through a single-step hydrothermal process. The synthesized composite was subsequently used to remove Methylene Blue from water and had a removal efficiency of 40 mg•g-1 with an adsorption time of 20 min. The adsorbed methylene blue was stabilized in the adsorbent through heat treatment, forming S- and N-doped carbon and improving the electrochemical properties of the final sample. The Methylene Blue stabilized composite yielded the highest specific capacitance of 426.5 F g-1 at 2 A g-1 among all in 3-electrode analysis. A device fabricated with this sample as cathode and carbonized grass as anode achieved a maximum specific capacitance of 98.3 F g-1 with a high energy density of 44.3 Wh kg-1 at a high-power density of 1.8 kW kg-1. The device also showed high capacitance retention of 97 % after 10000 charging-discharging cycles, which is excellent for practical applications.



Treatment of Heavy Metal Polluted Waste Water using Architectural Polymer Composites

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Abstract:

To meet the demands of potable, industrial and agricultural water there is a need to treat waste water. The impurities present in potable water can be in the form of suspended material, in the form of clay, silica, microbial organisms and inorganics. Moreover, the majority of industries such as paper and pulp, leather and tanning, paints and pigments, textile industries generate an enormous amount of coloured effluent and toxic heavy metals. Thereby, contaminants must be removed before they can be reused. Removal of heavy metal ions from wastewater is of prime importance for a clean environment and human health. Heavy metal-contaminated wastewater seeps into the environment, endangering human health and the ecosystem. They prove to be non-biodegradable and may be carcinogenic; thus, the presence of these metals in water by excessive amounts may cause serious health problems for living organisms. Even though these heavy metals can be detected in trace amounts, they are still dangerous and thus need to be removed. In this context, we would focus on the use of hyperbranched polymers for the adsorption of heavy metals owing to their irregular branched structures with a low degree of branching while retaining the desirable properties of dendrimers.

Optimization of Sr-modified bismuth molybdate semiconductor for highly efficient photoelectrochemical water splitting

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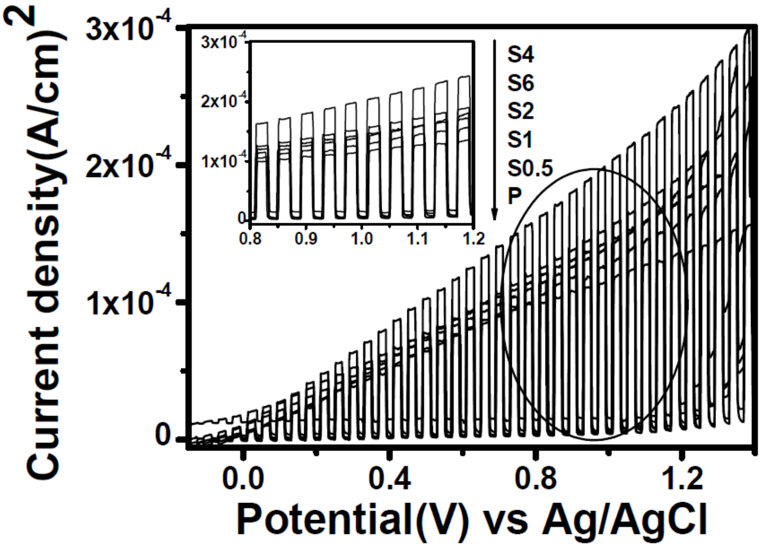
Abstract:

Bismuth molybdates are found to be very fascinating materials due to their narrow band gap energy, high chemical stability and suitable valence and conduction band potential, which makes them an excellent visible light active photocatalyst [1]. The heterostructure formation is regarded as a reliable strategy to achieve efficient charge separation and improved photocatalytic activity [2]. In this work, we have developed Sr modified bismuth molybdate thin film using a simple drop-cast method. The activity of the semiconductors was tested through LSV under chopped illumination in the presence of 0.1 M Na2SO4 and sulphite solution for water oxidation and sacrificial oxidation. The optimized thickness of Sr modified bismuth molybdate yields a photocurrent density of 281 μA/cm2 using LSV at 1.3V. In addition, the Sr modified bismuth molybdate photocatalysts maintained good stability for at least for an hour, most importantly, were visible light active.



Acknowledgement: The present work was financially supported by the Department of Chemistry, IIESTS.

Keywords: LSV, Electrochemical impedance spectroscopy, Stability

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Feasibility study of DNA-based porous membranes as gravity-driven purifications

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Abstract:

We demonstrate, the development of DNA-based stable porous aerogel membrane (PAMs) *via* a one-pot crosslinking reaction with genipin. Meanwhile, seaweed polymer agar was added during the fabrication of the porous aerogel membrane with the desired stability and porosity for sustainable water separations. Analyses of PAMs using advanced analytical tools (e.g., FT-IR, solid-UV, XPS, TGA and SEM). PAMs was tested for the separation of oil-water and hexane-water suspensions under gravity-driven force, which exhibits high rejection (~98%) with an excellent flux in the range of 332-389 L•m−2•h−1. PAMs were also tested for the separation of naphthalene from contaminant water with a good flux rate of 384 L•m−2•h−1. PAMs were reused for separation experiments in the next three cycles without any significant changes and they exhibited biodegradability under soil conditions. This work opens new areas of utilising biomolecule DNA to develop sustainable separation membranes in combination with seaweed polymers for gravity-driven filtration.

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Defluoridation of ground water by modified bentonite

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Abstract:

Prolonged use of fluoride contaminated drinking water causes serious health problems e.g., skeletal, and dental fluorosis. Upon treatment of 100ml 5ppm NaF Solution with 1g,2g and 3g modified bentonite up to 30 min, the concentration of fluoride decreased to 0.01 ppm. Similarly, 1g of modified bentonite on treatment with 100ml 5ppm NaF solution removed fluoride completely at a pH range 2-8. Bentonite has been modified by treatment of 15g, 300 mesh sieve bentonite with 500ml 100ppm Fe3+ solution. The removal of fluoride may be attributed to the high cation exchange capacity, layer structure and high surface area of bentonite. The experimental data fitted well to Langmuir isotherm model indicating a monolayer adsorption. The first order reaction kinetics was followed in the defluoridation by modified bentonite. This method may be adopted as an eco-friendly alternative of defluoridation because no free Al is released in water during the process.

Keywords:
Defluoridation , Langmuir isotherm, Modified bentonite, cation exchange capacity.

Efficient fluoride removal by magnesium zinc bimetallic oxide prepared by one-pot solution combustion method

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Abstract:

A novel porous spherical magnesium zinc binary oxide (MZO) was successfully synthesized for excess fluoride removal in drinking water by the one-pot solution combustion method. The adsorbent was characterized by XRD, FESEM, FTIR, and XPS. surface charge of the adsorbent was characterized by zeta potential. The prepared nano adsorbent showed a high fluoride removal capacity (43.10 mg/g). The adsorbent of fluoride was highly pH-dependent and effective between pH 6 to 9. The kinetic studies revealed that fluoride removal follows the pseudo-second-order rate law. Fluoride removal from groundwater is selective in presence of other co-anions like NO_3^-, Cl^-, SO_4^{2-} etc. It was found that the sample was quite reusable. XPS, FTIR, and zeta potential data indicate that the basic fluoride adsorption process of the material is related to ion exchange and electrostatic interactions. Thus, MZO could be treated as an efficient adsorbent for fluoride-containing groundwater to remove excess fluoride.

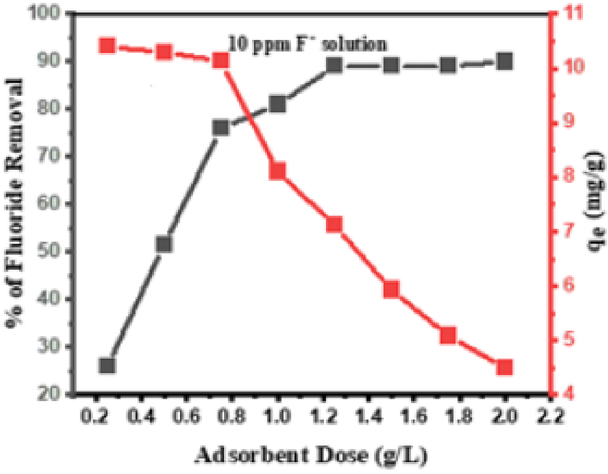

Fig1. % Of fluoride removal vs adsorbent dose

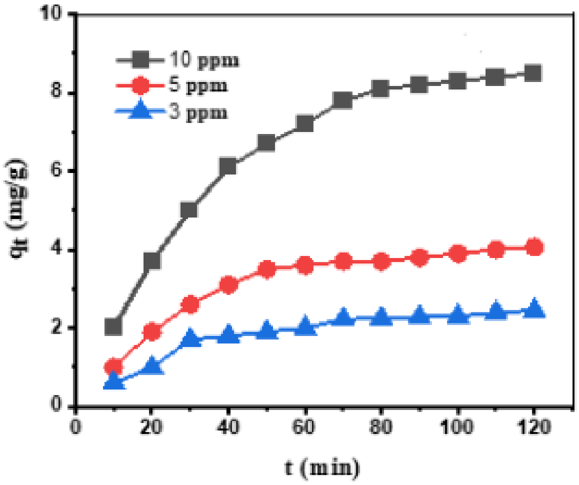

Fig 2. Adsorption kinetics

Efficient isolation of keratin from protein-rich waste biomass: a practical approach to minimize environmental impact and valorize waste biomass

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Abstract:

Among various protein-containing biomass wastes, waste animal wool, poultry feather, and human hair are considered one of the most important renewable sources of keratin. Animal wool and human hair are utilized for the production of several products. However, the substantial quantity of short fibres that are inappropriate for spinning and being unusable is thrown away as waste resulting in significant environmental issues in terms of their accumulation in water bodies resulting in obstruction of waterways and other related problems. Similarly, poultry wastes, especially waste chicken feathers (WCF) are dumped or burnt or used as low-value fertilizer in certain applications. This research aims to develop an efficient method to extract the recoverable keratin from various wastes thus isolated was established, and effectively utilize the spent solvent in the extraction process used for green gram (Vigna radiata) seed treatment, and significantly increase in the height and weight of the plants was observed. Treating biomass waste as a source of high-value compounds may minimize environmental impact by reducing the waste load.

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Prof. Suprakash Sinha Ray

Keeping Oxygen Out and Freshness In–A Novel Polymer Nanotechnology Approach to Food Packaging

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Caroline Mekoa[1], *Mpho Motloung*[1], *Vincent Ojijo*[1], *Suprakas Sinha Ray*[1,2]*
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Abstract:

Increased food insecurity has been a national point of concern due to the Covid-19 global pandemic, economic decline and climate change. Adding onto the list of concerns, is ineffective food packaging which compromises the quality of food. It is said, in South Africa, most losses and waste is estimated at 30% and occurs at the processing and packaging stage in the value chain. Using our advanced polymer formulation capability and our well-equipped Nanomaterials Industrial Development Facility, we were able to develop a nanotechnology-based solution which features a nanocomposite technology which will greatly benefit the industry. The technology is based on the incorporation of nano-minerals in polymers to deliver significantly improved barrier properties in a polymer film, which further improves the shelve life of food.

Suprakas Sinha Ray was born in 1973 in India and completed his PhD studies at the University of Calcutta in 2001, and then postdoctoral fellow at Toyota Technological Institute, Japan and Laval University, Canada studying the structure-property relationship in nano clay-containing polymer nanocomposites. He started working on fundamental understanding to real applications of polymer-based nanostructured materials when he joined (October 2006) the CSIR as a group leader. These studies advanced and broadened when he appointed as a chief researcher and founding director of the DSI-CSIR Nanotechnology Innovation Centre and growing to the present time with scientists, engineers, technologists, postdoctoral fellows, students, collaborators, and industrial partners worldwide. Currently, more than 115 researchers, engineers and technologists are working at the Centre.

He is one of the most active authors in the field of polymer nanocomposite materials and recently, he has been rated as a Top 1% of most impactful and influential scientists (Chemistry, Materials Science and 22 Science disciplines) by *Thomson Reuters Essential Science Indicators*. Prof. Ray is the author of 7 books, co-author of 5 edited books, 30 book chapters on various aspects of polymer-based nano-structured materials & their applications, and author and co-author of more than 500 articles. He also has 7 patents (registered or filled) and 10 new demonstrated technologies (commercialized) shared with colleagues, collaborators, and industrial partners. So far, his team commercialized 19 different products. Over the last 15 years, he has trained 23 postdoctoral fellows, produced 39 PhD and 23 Master students under his direct supervision. In 2016, he received South Africa’s *Most Prestigious National Science and Technology Award* (NSTF).

Prof. Tushar Jana

Polymers as Ion Exchange Membranes for Green Hydrogen Generation and Use

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Abstract:

The development of polymer-based ion exchange membranes (IEMs) with higher ionic conductivity, desirable mechanical strength, low acid leaching and high alkaline stability are the prime challenges to be achieved for the successful use of these membranes in various types of electrochemical devices such as fuel cell, water electrolyzer etc. Our group has developed several strategies to make IEMs from various polymers with a special focus on a class of polymers namely polybenzimidazoles (PBIs). Synthesis of tailor made PBI structures, development of a novel IEM fabrication process, blending of PBI with suitable polymers, and formation of PBI hybrid nanostructures are the few novel strategies so far, we have pursued to address the key challenges. I wish to discuss few examples arising from these approaches towards the development of PBI based IEMs and their application in high temperature proton exchange membrane fuel cell, water electrolyzer etc. I will also highlight an important recent result on the development of PBI based alkaline anion exchange membranes (AAEMs).

Few recent references:

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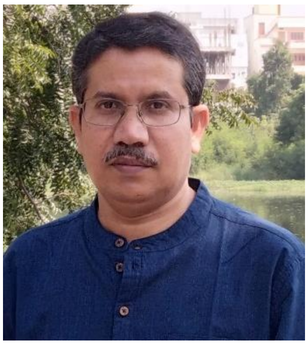
5. Harilal; Nayak, R.; Ghosh, P. C.; Jana, T. *ACS Appl. Polym. Mater.* **2020**, *2*, 3161.

For more deatils, vist us: **http://chemistry.uohyd.ac.in/~tj/index.html**



Prof. Tushar Jana received his B.Sc. (1995) & M.Sc. (1997) in Chemistry from University of Calcutta, Ph.D. in 2001 from the Indian Association for the Cultivation of Science (IACS)-Calcutta and worked as a postdoctoral researcher in University of Pittsburgh and Rensselaer Polytechnic Institute, USA during 2002-2005. He joined the faculty of the University of Hyderabad in 2005 and is serving as a professor of chemistry since 2013. He teaches various physical chemistry, materials chemistry and polymer chemistry related courses in the undergraduate and post-graduate levels. His research interests are focused in the areas of: *polymer membranes, polymeric nanostructures, and polyurethanes*. Prof. Jana has published ~ *100 research articles* in high impact international journals and holds *seven patents*, and his current *h-index is 36 with a total citation over 3700*. Prof. Jana is in the editorial board of PLOS One and Journal of Macromolecular Science, Part A: Pure and Applied Chemistry. Prof. Jana's achievements have been recognized with awards and honors which include Young Associateship from Indian Academy of Science, Young Scientist Medal from Indian National Science Academy and the Alkyl Amines-ICT Foundation Day Young Scientist Award from Institute of Chemical Technology, Mumbai, India. He has received University of Hyderabad Chancellor's Award (2018), Bronze Medal (2019) of Chemical Research Society of India. He is an Associate Fellow of Andhra Pradesh Akademi of Sciences. He has been elected as a Fellow of Telangana Academy of Sciences (2015), West Bengal Academy of Science and Technology (2021) and National Academy of Sciences, India (2022).

Prof. Dipankar Chattopadhyay

In-vivo evaluation of wound healing potency of electrospun biomimetic scaffold based on collagen crosslinked modified-chitosan and graphene oxide quantum dot nanocomposites

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Abstract:

Skin acts as a protective biological barrier between internal organs and the external environment. Inherently, the body can regenerate minor skin wounds in a spatially organized manner. However, critical sized skin injuries cannot be regenerated spontaneously and need external support. Therefore, different types of wound healing materials have been developed by exploring polymeric membranes, hydrogel, foam, sponges, and adhesive patches [1, 2]. However, most of the deployed conventional approaches could not successfully recover the critical wound area or accelerate the skin regeneration process effectively. Thus, there exists an urgent need for the development of efficient wound healing material with excellent biological properties to induce tissue regeneration at a rapid rate. An asymmetric scaffold was developed through electrospinning by utilizing biocompatible materials for effective wound healing applications. First of all, the chitosan surface was modified by decanoyl chloride and crosslinked by collagen to synthesize collagen crosslinked modified-chitosan (CG-cross-CS-g-Dc). Then, the asymmetric scaffold was fabricated through electrospinning, where the top layer is a monoaxial nanofiber of PCL/graphene oxide quantum dot (GOQD) nanocomposite and the bottom layer is a coaxial nanofiber having PCL in the core and CG-cross-CS-g-Dc/GOQD nanocomposite in the shell layer. The formation of monoaxial (~ 130 ± 50) and coaxial (~ 320 ± 40) nanofiber was confirmed by transmission electron microscopy (TEM). The presence of GOQD has contributed to antioxidant and antimicrobial efficacy. These scaffolds showed substantial antibacterial activity against regular wound pathogens, *Escherichia coli (E. coli)* and *Staphylococcus aureus* (*S. aureus*). The scaffold exhibited excellent cytocompatibility (MTT assay) and anti-inflammatory behaviour as analysed via cytokine assay and biochemical analysis. The in-vivo wound healing potential of the nanofibrous scaffolds was assessed with the assistance of full thickness excisional wounds in the rat model. The scaffold accelerated the re-epithelialization as well as the collagen deposition, thereby facilitating the wound healing process in a very short span of time (10 days). Both *in vitro* and *in vivo* analysis thus provides a compelling argument for the therapeutic biomaterial and its suitability in rapid wound regeneration and repair.

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Prof. Dipankar Chattopadhyay is currently a Senior Professor at the Department of Polymer Science and Technology, University of Calcutta. He joined this department in the year 2006. Before that, he obtained his Ph. D degree from Polymer Science Unit, Indian Association for the Cultivation of Science, Jadavpur, India. He has got B.Sc. (Chemistry) and B.Tech. (Plastics & Rubber Technology) from Ramkrishna Mission Vidyamandira, Belur Math and Department of Polymer Science and Technology, University of Calcutta. He has obtained M.Tech. (Polymer Science and Engineering) from the Department of Polymer Science & Engineering, Indian Institute of Technology, New Delhi, India. He is an industrial consultancy expert for reputed companies such as Exide Industries Ltd., Philips Carbon Black Pvt Ltd., PSG Institute of Advanced Studies (CARS Program), Amer-SilKetex Pvt. Ltd. Etc. He has completed 8 research projects with total funding of 1.0196 cores funded by different funding agencies such as CU, CSIR, DST, DBT, WBDST, Tata Steel, etc. Two projects with total funds of 35 lakhs are ongoing. He has guided 16 Ph. D students and 10 Ph. D students are working under his supervision. He has published 160 research articles in the international journals of repute and several book chapters (h-index-40, i-10 index 116). He has obtained three patents jointly with Tata Steel. He is fellow of West Bengal Academy of Science and Technology. His name is listed in the Stanford 2% list of Scientists Globally for consecutive two years.

His Research Areas of Interest are:

- Nanostructured conducting polymers for sensing,
- Nano metals and metal oxides for antimicrobial coatings of fabric,
- Graphene and Clay based composites,
- Transdermal and ophthalmic drug delivery.
- Adsorption for water treatment,
- Nanocrystalline cellulose based composites with rubbers and plastics,
- Thinned layer 2D transition metal dichalcogenide (i.e. MoS_2, WS_2, $MoSe_2$, etc.) for energy harvesting applications,
- Halide-free metal perovskite nanocrystal for supercapacitor applications
- Thinned layer 2D Mxene for supercapacitor applications,
- Devulcanization of rubbers.

Prof. Santanu Chattopadhyay

Doped nanohydroxyapatite incorporated polyurethane-urea based porous scaffolds for accelerated bone regeneration: A judicious approach

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Abstract:

In modern civilization the increasing number of bone defects, caused by uncontrolled lifestyle, diseases, congenital effects, or accidental fracture urge to formulate a promising strategy to repair the defected bone. However, the slow rate of auto osteoinduction, improper osteo-reconstruction, and bacterial colonization at the fracture site are the foremost reasons for developing significant approaches to augment bone regeneration. Though the allografts and the autografts are the gold standard grafting strategies for treating bone defects, additional second site operation, scarcity of donor site, high risk of infection, and immune rejection limit them as bone grafting techniques in practical biomedical applications. Recently, polymer-based porous bone graft substitutes using modern techniques like electrospinning and 3D printing are widely used in bone tissue regeneration. To enhance the osteogenic bioactivity, different osteoconductive nanomatrerials like carbonaceous nanomaterials and transition metal-based nanomaterials are introduced along with the bone mimetic nanomaterial nanohydroxyapatite (nHA) within the polymer matrix. The carbonaceous or the transition metal-doped nanohybrid materials (functionalized carbon nanotube doped nHA or titanium phosphate doped nHA) was prepared judicially and incorporated within the synthesized biomolecule tethered segmented polyurethane-urea (SP) to fabricate the porous scaffolds. The incorporation of minute amount (0.15%) of carboxyl functionalized multiwall carbon nanotube (CCNT) along with nHA improves the tensile strength and the hardness of the nano-scaffold by 94.5% and 173.6%, respectively. Moreover, the surface bioactivity of the fabricated scaffolds was enhanced by the immobilization of biomolecule polydopamine (PDA) on the surface of the scaffolds. The incorporated transition metal with its high effective nuclear charge (Z*) and small ionic radii interact strongly with the catechol group of dopamine which increased the PDA deposition on the surface of the scaffolds. The nanohybrid scaffolds with a higher amount of deposited PDA with active surface functional groups (hydroxyl and amine groups) increase the surface wettability of the scaffolds. The higher amount of immobilized PDA with active functional groups can bind various growth factors, enzymes, and proteins in exact physiological media which facilitates faster cell adhesion, proliferation, and osteogenic bioactivity of the scaffold. Thus, a minute amount of CCNT and transition metal doped nHA incorporated segmented polyurethane-urea based micro-porous nanohybrid scaffold with improved physicochemical properties and osteogenic bioactivity could be utilized as an excellent advanced material for bone regeneration substitute.

Prof. Santanu Chattopadhyay is currently the Professor of Rubber Technology Centre, Indian Institute of Technology Kharagpur, India. He has been serving there as a Faculty at IIT Kharagpur there since 2004. Prof. Chattopadhyay has pursued his post-doctoral research work in Georgia Institute of Technology, USA from Chemical Engineering & Biomolecular Engineering working with Prof. Carson Meredith in the year 2002-2004. Prior to that he did his post-doctoral studies as well in the University of Western Ontario, Chemical & Biochemical, Engineering, Canada for one year working with Prof. Judit Puskas on cationic polymerization and synthesis of isobutylene based TPEs. Prof. Chattopadhyay did his PhD from IIT Khargpur in 2001 working with Prof. Anil K. Bhowmick on Thermoplastic Elastomer Blends as shape-memory materials. Prior to these, he did his M.Tech. (Materials Science) working with Prof. M.V. Pandya, IIT Bombay and M.Sc. (Chemistry) from IIT Kharagpur.

He has published more than 175+ papers in international journals, (out of which more than 10 publications having 10+ impact factors) 150+ conference proceedings, about 10 book Chapters and a few patents. His research interests include Biopolymers and Polymers in Healthcare, Viscoelasticity and Processing of rubbers, Tapping Energy from Rubbery Materials, Green & Sustainable rubbers and compounds, Smart and Advanced Materials, Die and Mold design (CFD) and FEA & MD Simulation & Design of Rubber Products. He has completed supervising 22 PhD students and 55+ master's student so far and currently supervising 18 PhD students in various facets of Biopolymers, Polymer Science and Rubber Technology. He has been offering constancy and actively pursuing several sponsored industrial researches for various Rubber Industries and Government funding agencies of India and Abroad.

Dr. A.K. Mukherjee

Novel reagents in Mineral Processing and Agglomeration

Dr. A.K. Mukherjee
Chief, Raw Materials Research Group, Tata Steel R&D, Jamshedpur.

Abstract:

Several reagents including polymers, composites, surfactants, inorganic salts and organic materials find potential application in the field of mineral processing and agglomeration. High molecular weight, water-soluble polyacrylamides and related products have for many years, been used successfully within the Mineral Processing Industry to aid solid-liquid separation. Organic surfactants and reagents have been used as collectors in iron ore and coal flotation. Recently, organic polymers and composites are received significant attention as binders for iron ore pelletization and sintering. This traditional area of use is discussed with particular emphasis being placed upon the more recent innovations in terms of equipment and modifications. Other areas of application include dispersants and to a much lesser degree binders and dust suppressants. Furthermore, a portion of the research is devoted to the role of the latest addition to the polyacrylamide group of products - water absorbent polymers. To address the increasing complexity of mineralogy, new reagents in minerals processing are highly sought after, hence the need to understand and develop materials for improving selectivity and functionality is the need of the hour.

Dr. A.K. Mukherjee

On completion of my studies at ISM Dhanbad joined IREL (a company under Dept. of Atomic Energy). A tenure of little more than 7 years at IREL provided me the exposure to plant problems related to processes and quality. With this experience joined R&D Division of Tata Steel and started learning to solve process issues from first principle. This was further nurtured through the Ph.D program at IIT Kanpur (2003 – 07). My Ph.D work has been focused on fundamental investigation into particle segregation during jigging and its industrial application. We developed a control strategy and the same was applied to a 300 tph capacity jigging plant that was under commissioning at Noamundi. To probe the segregation process at particle level, a numerical tool based on the Discrete Element Method (DEM) was used. In the Indian context, our work contributed towards the changing scenario in iron ore processing. Today, several companies are contemplating jigging as an option to treat medium – grade iron ore which was perhaps unthinkable just two decades ago. In the subsequent years, my research experience and the ability to collaborate with national and international agencies (which includes premier national institutes, Chinese University, US agency and AMIRA – a largest consortium in mining domain), had yielded completion of successful big projects such as iron ore slime beneficiation, Dense Media Cyclone design, Column flotation sparger design, LD slag beneficiation etc.

My work was recognised at national level through awards such as National Mineral Award (the highest award by the Ministry of Mines, Govt. of India) and IIME Mineral beneficiation award (a peer group award). At Tata Group level, these works were appreciated by the Tata Innovista award and at Tata Steel level by the best project award (3 times) and best paper award. Furthermore, my research work had helped me to develop contacts at international and national level. Presently, I am a member of the international body (International Mineral Processing Congress), an adjunct faculty to CSIR, review committee members of projects under ministry of Mines and reviewer of few international journals.

Prof. Sudip Malik

Applications of Conducting Polymer Nanotubes: Water Purification, Energy Storage and Memory Switching

Prof. Sudip Malik
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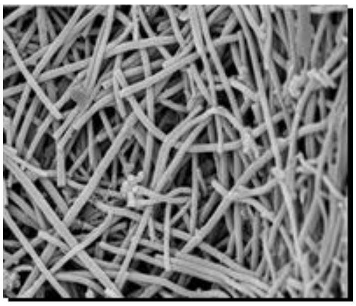
Abstract:

Conducting polymer (CP) nanostructures have received more attention nowadays owing to the success of getting defined size, shape, architecture and chemical functionality, as a result, CPs are the forefront of many next-generation organic optoelectronic technologies. Among CPs such as polypyrrole, polythiophene, polyphenylenevinylene, and polyacetylene, polyaniline (PANI) has been most extensively studied because it shows good environmental stability and its electrical properties can be modified by both the oxidation state of the main chain and protonation. However, the control of the size and morphology during the synthesis of nanostructured PANI still remains a challenge. Inspired by the easy preparation of PANI and the use of water as an environment friendly solvent, we wonder if we could directly obtain nanoscale PANI in aqueous medium. Herein, the current lecture will discuss about the structure and properties of CPs in general, particularly the formation of CP nanotube (below picture) and the recent applications of these nanotubes.



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Chem. C, 2014, 2, 3382–3389.
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9) P. Das, S. Mondal and S. Malik, J. Energy Storage, 2021, 39, 102662.

1. **Broad Area of Research**: Design and synthesis of novel oligomers, polymers and self-organizing systems and the subsequent observation of their structure-property relationships.

2. **Professional Records**:
2021-present Senior Professor: SAIS / IACS / Kolkata /INDIA
2018 – 2021 Professor: SAIS / IACS / Kolkata /INDIA
2013 – 2018 Associate Professor: PSU / IACS / Kolkata /INDIA
2009 – 2011 **Marie Curie Fellow**: Radboud University of Nijmegen, NETHERLANDS (on leave from IACS).
2008 – 2013 Assistant Professor: Polymer Science Unit (PSU) / IACS / Kolkata /INDIA
1998 – 2003 PhD Jadavpur University / IACS / Kolkata /INDIA

3. **Honours / Awards/ Distinctions / Prizes Received**:

2000	CSIR Fellowship, New Delhi, Govt. of India
2005–2007	**JSPS Fellowship**, Kyushu University, Japan
2009–2011	**Marie Curie Fellowship** (International Incoming), Radboud University of Nijmegen, Nijmegen, The Netherlands
2009–2012	**Young Associate of Indian Academy of Sciences**, Bangaluru, India
2022	**12th Polymer Foundation Award**, Prof. S. Maiti Polymer Foundation Award

Number of Publication: 90
Number of Patent: 2
Number of Book Chapter: 5
Number of PhD thesis guided : 11(+7 ongoing)

4. **Current Research / Development Activities**:

I. Conducting Polymer Nanostructures for Energy Application.
II. Design and Synthesis of Polyfluorene Copolymers for Sensors or Solid-State Emissive Materials
III. Small Molecular Aggregation and Hydrogelation.
IV. Intercalation of chromophores or polymers into Nanoclay.
V. Electrochromism and Smart Window.

Prof. Nikhil R. Jana

Controlling the Intracellular Processes via Chemically Designed Nanoparticle

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Abstract:

In past few decades there is significant advancement in biomedical applications of various nanoparticles. Current chalenges include designing nanoparticle that can readily cross the cell membrane, target different subcellular compartments and control intracellular processes. We design colloidal nanoparticle/nanobioconjugate of 10-50 nm size and use them to control various cellular processes. We found that cellular uptake and intracellular function of nanoparticle can be controlled by appropriately designed surface chemistry. We show that nanoparticle can be designed for energy independent direct cell translocation (without endocytosis) or preferencial lipid raft/caveolai-mediated endocytosis as compared to conventional clathrin-mediated endocytosis. Adapting these principles we design nanoprobes that can readily enter into cell, label different subcellular compartments, inhibit intracellular protein aggregation and clear toxic amyloid aggregates via upregulated autophagy. The talk will focus on property of our designed nanoprobes along with various application potentials.

Reference:

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3) Dolai, J.; Mandal, K.; Jana, N. R. ACS Appl. Nano Mater. 2021, 4, 6471-6496.
4) Debnath, K.; Sarkar, A. K.; Jana, Nihar R.; Jana, Nikhil R. Acc. Mater. Res. 2022, 3, 54-66.

Education:
BSc: Midnapore College
MSc: IIT-Kharadpur
PhD: IIT-Kharadpur
Postdoc: University of South Carolina and University of Arkansas, USA

Awards& Honours:
1) Materials Research Society of India (MRSI) Medal, 2015
2) Member, Editorial Board, ACS Applied Materials and Interfaces, 2016 - 2019
3) Fellow, West Bengal Academy of Science & Technology (FAScT), 2016
4) Associate Editor, ACS Applied Nano Materials since 2019

A brief introduction about your academic and research..........................

Professor Nikhil R. Jana received his PhD in chemistry from Indian Institute of Technology-Kharagpur in 1994. He was a postdoctoral fellow at University of South Carolina (1999-2001) with Professor Catherine J. Murphy and at University of Arkansas (2003) with Professor Xiaogang Peng.

He moved to Singapore in 2004 and worked as a Scientist at the Institute of Bioengineering and Nanotechnology, until he returned to India in 2008 and began his independent research carrier at Indian Association for the Cultivation of Science (IACS). He is currently Sr. Professor at School of Materials Science at IACS.

His laboratory focuses on chemical synthesis of colloidal nanobioconjugate and their application as bioimaging nanoprobe and for prevention/curing of neurodegenerative diseases. He has authored or co-authored more than 180 peer-reviewed articles and 2 books on basic and applied science, with a primary focus on tuning of nanoparticle surface chemistry toward various biomedical applications.

Prof. Sanjay Kumar

An Overview on Potential of Designer Organic Co-crystal and Salts as Organic Semiconductors

Sanjay Kumar
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Abstract:

Among two elemental semiconductors (Si and Ge), silicon is the primary ingredients for fabricating semiconductor devices and ICs (chips). Currently, the silicon chips are embedded in almost all day-to-day used gadgets but those are manufactured by the cost of very high carbon footprint. For example, a single 700 acre fab of Intel at Ocotillo, Arizona in a month, consumes ~ 200 m-kWh of energy electricity and 300 m-gallons of water and discharges 5000 tons hazardous waste and contaminated water. In this context, the organic semiconducting materials have emerged as a viable alternative of Si. Organic semiconductors (OSCs) are eco-friendly and possess some appealing features like ease of synthesis procedure and processing ability at room temperature, abundant availability, lighter weight, low production cost, and remarkable mechanical flexibility. Till date, the market domain of OSCs (used in low power relatively slow foldable or flexible electronic devices) and Si is mutually exclusive. In the 1970s, Heeger, Shirakawa, and MacDiarmid have shown that the conductivity of polyacetylene can be enhanced to a level of metal upon exposer to chlorine, bromine, or iodine vapour, for which they have been awarded with the Nobel Prize in the year 2000. This has busted up the research on OSCs to a large extent. Since the invention of organic thin film transistors (OTFTs) the OSC technology has started blooming. Nowadays, the OSCs are commercially used in flat panel liquid crystal displays (OLCDs), active-matrix organic light-emitting diode displays, (AMOLEDs), OLED lighting, organic photovoltaic cells, smart cards, radio-frequency identification tags (RFID), tracking devices, sensor arrays such as electronic noses responsive to different organic odours. As of now the global market size of OSCs chips is USD 179.4 billion (2022) and is expected to exhibit a CAGR of 22.4% during 2019-2024.

The oligoacenes (like pentacene), oligothiophenes and fullerenes are extensively studied OSCs (both as thin film and single crystal) as they have enormous applications in fabrication of electronic devices. The basic designee principle to be followed and future prospect of OSCs are embedded in two enlightening statements one made by Richard Feynman, the great visionary who told: “What would the properties of materials be if we could really arrange the atoms the way we want them?” and another of Professor Heeger, who commented: “I’m convinced that we are on the verge of a revolution in ‘Plastic Electronics.” in their Nobel lecture. Plethora of semiconducting multicomponent organic cocrystals and salts demonstrating better transport and optoelectronic properties than single component OSCs have been designed by utilizing crystal engineering principles. Interestingly, the perylene-TCNQ cocrystal with the stoichiometry of perylene:TCNQ = 1:1, acts as n-type semiconductor with electron mobility of 10^{-3} cm2 V^{-1} s^{-1}, while the perylene:TCNQ = 3:1 behaves as p-type semiconductor with a hole mobility of 10^{-4} cm^2 V^{-1} s^{-1}.Clear understanding of intermolecular interactions, supramolecular synthons and recognition of events are the key factors for designing organic semiconducting cocrystals/salts with engineered band structure, available sites for carrier generation and pathway for carrier transport upon application of electric field. Given this background, the present lecture will be focused on (i) some of the seminal works on

OSCs and (ii) the study of crystal structure, band structure, thermal property, spectral behaviour of some multicomponent organic cocrystals/salt along with electronic transport property and optoelectronic response of those cocrystals/salt based Schottky barrier diodes reported by us.

Research Profile

Previous area of Interest:

Application of Nuclear Techniques in Condensed Matter Physics

Broad Area of Interest:

Experimental Condensed Matter Physics and material Science

Specific Area of Research:

1. Nano-magnetism
2. Molecular magnetism (single molecule magnet single chain magnet)
3. Magnetic and hyperfine (Mossbauer spectroscopy) properties of ferrites
4. Supercapacitor electrode material, sensing (bio molecules)
5. Catalysis & photocatalysis
6. Crystal Engineering (Designer Metal Organic Framework, Covalent Organic Framework, Hydrogen Bonded Supramolecular Framework, Organic Semiconductor)
7. Transport and Dielectric Properties.

Contribution to Research

Thesis title: Study on some iron based compounds and alloys byMössbauer spectroscopic.

Ph. D supervisor: Prof. D. Banerjee, Sir Rashbehari Ghosh Professor, Department of Physics, University of Calcutta & Mentor: Prof: Rangalal Bhattacharya, Professor, SINP & Department of Physics, University of Calcutta.

No. of Publication in International Journals: 109

h-index: 24

i10 index: 54

Last 5year i10 index: 43

No. of Doctoral thesis guided:

(i) Awarded: 13,

(ii) Registered: 08,

Sponsored Project Supervised: 2,

Invited lecturers delivered: 15

Recognition: Ranked among top 2% Scientists, by Stanford University in year 2021

Dr. Ambar Baran Bhowmik

Industrial PTA Manufacturing Process & Technology

Ambar Baran Bhowmik
MCPI Private Limited
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Abstract:

An overview of commercial manufacturing process of PTA (Purified Terephthalic Acid) has been described in the presentation. PTA contains over 99.99% (by weight) of Terephthalic Acid (TA) and less than 25 ppm of 4-Carboxybenzaldehyde (4CBA) and nearly 150 ppm of *para*-Toluic Acid (p-TA). Large scale production of PTA has two stages: in the 1st stage para-Xylene is oxidized to form Crude Terephthalic Acid (CTA) which is having high impurity level (around 3000 ppm of 4-CBA & trace amount Benzoic Acid, BA etc.). In the 2nd stage CTA is refined to PTA. PTA is the key raw material for the manufacture of polyester fiber, resin & film. PTA is consumed in processing polyethylene terephthalate (PET). Worldwide around 65% of PTA goes into polyester fiber, 27% to PET bottle resin & the remaining 8% to film and other plastic end users. In this presentation, the main focus is given to the steps of industrial large-scale production of PTA process & technology including the chemical reaction, unit operations involved.

Dr. Ambar Baran Bhowmik

Permanent address: B-11/39, Kalyani, Nadia, West Bengal, Pin: 741235.
Present Address: MCPI Private Limited, Haldia-721635. (Corporate Office: Bengal Eco Intelligent Park, Tower-1, 3rd Floor, Block-EM, Plot No. 3, Salt Lake City, Sector- V, Kolkata- 700091), West Bengal, India.
Vice President- MCPI Private Limited.
Head of Production-Technology-Project-Logistics & Quality division.
Nearly 25 years of experience in management of PTA plant
Operation, Design, Construction, Commissioning, Stabilization, Debottlenecking activities.
Overseas Assignments: Two years deputation: Technology & Development Center of Mitsubishi Chemical Corporation (MCC), Kurosaki, Japan.
Short assignments: Compressor- Gas Turbine- Steam Turbine division in Siemens Germany, PTA plants in China, Indonesia, South Korea etc.
Bachelor of Chemical Engineering (First Class Honours),
Jadavpur University, Kolkata, West Bengal, in the year 1998.
Date of Birth: 29th April 1974.

Prof. Pralay Maiti

Sustainable Polymers in Energy Sectors

Pralay Maiti, *Shivam Tiwari, Om Prakash, Ravi Prakash, Sunil Kumar*
School of Materials Science and Technology, Indian Institute of Technology (BHU),
Varanasi 221005
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Abstract:

Sustainable use of materials is need of the hour especially in energy sector due to huge demand in power supply globally. Polymeric materials are good choices mainly because of easy processing, specific properties, light weight and cost effectiveness. We develop a radiation resistant polymer by dispersing a few weight percentages of nanoparticles in the matrix polymer. Chemical changes due to SHI irradiation have been illustrated comparing the influence of nanoparticles dispersed in to PVDF matrix. Molecular level changes after irradiations have been confirmed by using spectroscopic, sol-gel technique and *in-situ* residual gas analysis. Chemical modification of nano-channels improves the conducting behaviour of insulating polymer into semi-conducting membrane. The membranes have been used to fabricate the fuel cell assembly and found a cheaper membrane as compared to commercially available Nafion. Developed piezoelectric materials are used for energy harvesting purpose. Solar cell devices have also been fabricated using the suitable materials, through the suitable energy diagram, and found significantly high-power conversion efficiency. Modified polymers are also demonstrated in energy harvesting by utilizing waste mechanical resources, waste materials and quantum dots as active material.

References:

K. K. Jana, A. Srivastava, O Parkash, D.K. Avasthi, D. Rana, V. K. Shahi, P Maiti *Journal of Power Sources* 301, 338 (2016); 2) K. Jana, A. Thakur, V. K. Shahi, D. Avasthi, D. Rana, P. Maiti *Journal of Materials Chemistry A* 3, 10413 (2015); 3) K. Jana, C. Charan, V. K. Shahi, K. Mitra, B. Ray, D. Rana, P. Maiti *Journal of Membrane Science* 481, 124 (2015); 4) K. K. Jana, N. K. Vishwakarma, B. Ray, S. A. Khan, D. K. Avasthi, M Misra, P. Maiti *RSC Advances* **3**, 6147 (2013); 5) K. K. Jana, B. Ray, D. K. Avasthi, P. Maiti *Journal of Materials Chemistry* 22, 3955 (2012); 6) V. K. Tiwari, T. Shripathi, N. P. Lalla and Pralay Maiti *Nanoscale* 4, 167 (2012); 7) V. K. Tiwari, D. K. Avasthi and P. Maiti *ACS Applied Materials and Interfaces* 3, 1398 (2011); 8) O. Prakash, A. M. Mhatre, R. Tripathi, A K. Pandey, P. K. Yadav, S Khan, and P. Maiti *ACS Applied Materials & Interfaces* 12, 17628 (2020); 9) R. Prakash, I. C. Maurya, P. Srivastava, S. Mondal, B. Ray, P. Maiti *Nanoscale Advances* **4**, 1199 (2022).

Dr. Pralay Maiti is currently a senior professor and ex-coordinator in the School of Materials Science and Technology, IIT (BHU), Varanasi. Prof. Maiti has received his Master in Chemistry from Indian Institute of Technology, Kharagpur in 1991 and Ph.D. in Polymer in 1996 from The Indian Association for the Cultivation of Science (Jadavpur University). He was COE Researcher and Lecturer at Venture Business Laboratory, Hiroshima University, Japan (1997-1999) and was post-doctoral fellow at Toyota Technological Institute, Japan (1999-2001). He was Visiting Scientist at Cornell University, USA from 2002 to 2004. He was Quick Hire Fellow at Central Leather Research Institute, Chennai before joining the School of Materials Science and Technology as Reader in December 2004. His current research interests include drug delivery vehicle, biomaterials, and energy materials.

Most innovative contribution of Prof. Maiti is in the field of materials chemistry related to drug delivery using biodegradable polymers, self-assembly and energy materials through nanotechnology and their uses in energy sector. He has published more than 200 papers in high impact peer reviewed journals, 22 patents (few of them are commercialized) and 27 book chapters. Prof. Maiti is the recipient of many awards like National award for Technology Innovation, APA Young Scientist award, Prof. Santappa silver jubilee medal, NASI-Reliance platinum jubilee award, Tata innovation fellowship are few of them.

Dr. Tarun Kumar Mandal

Side-Chain Functional Polypeptides: Stimuli-responsiveness, Aggregation and Application

Tarun K. Mandal
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E-mail: *psutkm@iacs.res.in*

Abstract:

Side-chain functional polypeptides and their aggreagtes are gaining increasing interest as potential bio-inspired materials for various appliactions. Inspite of their inherent biocompatibility and biodegradability, the hydrophobic nature of polypeptide moieties restrict their use in biomedical applications including delivery of drug, gene etc. Thus, our research is focoused on the preparation of functionalized polypeptides with various hydrophilic polymers and ionic groups to increase their water solubility, particularly to introduce different stimuli-responsive properties. Our recent achievements on several different techniques for functionalization of polypeptides will be discussed. Poly(2-oxazoline)s are known to be pseudopeptidic bio-inspired water-soluble thermoreponsive polymers. Thus, the motivation is to integrate poly(2-oxazoline)s with different reactive polypeptides prepared using ROPs and CuAAC "click" techniques to make thermoresponsive polypeptide copolymers with high propensity to self-assemble into micellar/vesicular nanostructures for various potential applications including encapsulation of dyes/drugs and their control release. The technique to prepare water-soluble ionically functionalized polypeptide will also be discussed by ring-opening polymerization (ROP) of a functionalized amino acid-based N-carboxyanhydride (NCA) monomer followed by the nucleophilic substitution reaction. ROP to synthesize photoresponsive positively charged polymethionine and its block copolymer, followed by post-functionalization through nucleophilic substitution reaction will also be discussed. The discussion will also focous on the ion-induced thermo-responsiveness of these ionically functionalized polypeptides in water along with its DNA-binding capability and photo-tiggered release.

References

[1] Dinda, P.; Anas, M.; Banerjee, P.; Mandal, T. K., *Macromolecules* **2022**, 55, 4011-4024.
[2] Anas, M.; Dinda, P.; Kar, M.; Mandal, T. K., *Polym. Chem.* **2021**, *12*, 6329-6343.
[3] Anas, M.; Jana, S.; Mandal, T. K., *Polym. Chem.* **2020**, *11*, 2889-2903.
[4] Jana, S.; Biswas, Y.; Mandal, T. K., *Polym. Chem.* **2018**, *9*, 1869-1884.
[5] Bose, A.; Jana, S.; Saha, A.; Mandal, T. K., *Polymer* **2017,** *110***,** 12-24.

Tarun K. Mandal received his B.Sc. and M.Sc. in Chemistry from University of Calcutta, Kolkata. He completed his Ph.D. from Indian Association for the Cultivation of Science/Jadavpur University, Kolkata, India in 1997. After two successive postdoctoral stays at National Cheng Kung University, Taiwan, and Tufts University of USA, he joined Polymer Science Unit, Indian Association for the Cultivation of Science, Kolkata, India in 2001 and subsequently served as Associate Professor and Professor in the same department. From 2014, he has been a Senior Professor at the Polymer Science Unit and served as the Head of this Unit of IACS (2009-2012). Presently, he is a Senior Professor at School of Chemical Sciences.

He is a recipient of the Materials Research Society of India Medal (2012) and the Chemiacl Research Society of India Bronze Medal (2013). He is a fellow of West Bengal Academy of Science and Technology since 2014. He has received M. Santappa Award in Polymer Science in 2018.

Professor Mandal has made significant contributions in various areas of polymer chemistry and materials science, which include the use of controlled polymerization techniques to synthesize stimuli-responsive polymers, peptide-polymer hybrid nanostructures, mesoporous polymers, amino acid-based polymers, functionalized polypeptide, metal/metal oxide-polymer hybrids for exploiting them in diversified range of applications from advanced materials to catalysts.

He has supervised 16 students for obtaining their Ph.D. degree and few students are working at various stages of their PhD. He has published more than 120 articles in highly reputed international journals, which have more than 5590 citations. His peers have recognized his contributions by citing his publications; his present *h*-index is 36.

Homepage: *http://iacs.res.in/athusers/index.php?navid=0&userid=IACS0083*

Prof. Biswajit Ray

Induction of Chirality in Polymers *via* Controlled Radical Polymerization using Natural Product Based Chiral Initiators

Biswajit Ray

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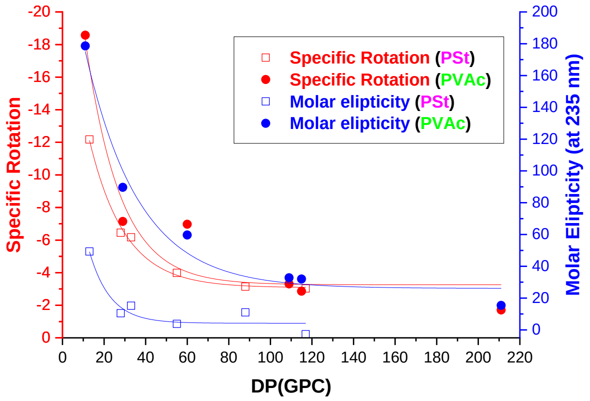
Abstract:

Naturally available L-Menthol-based atom transfer radical polymerization (ATRP) initiators and reversible addition-fragmentation chain transfer (RAFT) agents have successfully been synthesized and used for the controlled radical polymerization of styrene (St) and vinyl acetate (VAc), respectively.[1,2] Using these methods, two series of L-Menthyl-tagged two different polymers, polySt (PSt) and polyVAc (PVAc), having different molecular weights with low PDI have been synthesized and characterized by ^{1}H NMR, GPC, UV, polarimeter, CD, TG-DTA, and DSC studies.[3] Polarimetric and CD studies have revealed that specific rotation and the molar ellipticity at 235 nm magnitude decreases exponentially with increase in the molecular weiht of PSt and PVAc polymers. No effect of terminal L-Menthyl group on the stereoregularity of all formed polymers having different molecular weights has been observed. T_g of both polymer series increases exponentially with the increase of their molecular weights. Thus, we conclude that living radical polymerization using a suitable ATRP initiator or, RAFT agent containing a suitable chiral moiety can be useful in inducing chirality in a polymer up to high chain length. Choice of a suitable chiral moiety may increase the magnitude of chiral induction as well as induce chirality up to longer chain length of a polymer.



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[1] Vishwakarma S., Kumari A., Mitra K., Singh S., Singh R., Singh J., Sen Gupta S. K., Ray B. *J. Applied Polymer Science*, **2019,** *136(38)*, 47964.
[2] Vishwakarma S., Kumari A., Mitra K., Singh S., Singh R., Singh J., Sen Gupta S. K., Ray B. *J. Macromolecular Science, Part A*, **2020,***57(4)*, 299–309.

Prof. Biswajit Ray

Education: (i) B.Sc.(H) (1986-1989) & M.Sc. (Physical Chem Spl.) (1990-91) (Calcutta University); (ii) Ph.D (1992-1998) (Worked at Indian Association for the Cultivation of Science, Jadavpur, Kolkata with Prof. Broja Mohan Mandal and received degree from Jadavpur University)

Research Experiences: (i) Post-doctoral Fellow at Dept. Of Chemistry, Technion-Israel Institute of Technology with Prof. Moris S. Eisen (1999-2000), (ii) CNRS Researcher at Institute of Charles Sadron, France with Prof. Jean-Michel Guenet (2000-2001), (iii) JSPS Fellow at Dept. Of Chemistry, Nagoya University with Prof. Yoshio Okamoto (2002-2004), (iv) JST researcher at Dept. Of Chemistry, Osaka City University with Prof. Shigeru Yamago (2004-2005)

Professional Affiliations:

2005 - Joined as Reader at Department of Chemistry, Faculty of Science, Banaras Hindu University.

2008 – Become Associate Professor at the same department

2011 – Become Professor at the same department

Project Undertaken as PI /Co-PI:

Projects completed as PI: 4 (two CSIR and one DST and one DBT);
Projects completed as Co-PI: 1 (DIT)

Teaching Experiences: Basic Physical Chemistry courses of graduation and post-graduation level, Materials chemistry and Polymer chemistry courses.

Research Interests: Controlled synthesis of polymer, Stereo-regular polymer/gel synthesis, Graphene-based polymer composites, Biomaterials, polyurethanes, metal nano-particle synthesis, graphene quantum dot synthesis, carbon dot synthesis etc.

No. Ph.D. Students: 13 (awarded degree);1 (submitted) 2 (working)

No. of Publications in Peer Reviewed Journals: 98

No. of Patents: 1

Membership: (i)Life member, Polymer Science Society of India; (ii) Life member, Chemical Research Society of India; (iii) Member, American Chemical Society, (iv) Life member, Asian Polymer Society.

Dr. Jhuma Ganguly

Functionalized Microgel

*Dr. Jhuma Ganguly**
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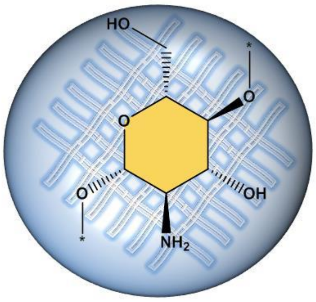
Abstract:

Microgels are assembled networks of colloidal size and withhold solvent molecules in structural interspatial in gel form. Functionalized gels are obtained from grafting of cross-linker moieties in natural macromolecules such as, e.g., polysaccharides, peptides or synthetic polymeric backbone. The extent of incorporated cross-linkers could be a way to regulate their cross-linked networks either gel or colloidal or macromolecular states. The mechanism of chemical bonding within gel-networks is very significant and interesting study to explain insight view as native or with change of solvents. This structural diversity and chemical association help to improve their potentialities for mechanical, fluorescence, flexibility, binding with protein, drugs and blood transportation supports in various applications. The porous and stimuli-responsive biogel materials could be better substituents of risky synthetic polymeric materials.



References:

1. Jana, B., Pan D., Chatterjee, A., Parshi, N., Ghorai S., Chakraborty, N., Ganguly, J., *ACS Appl. Polym. Mater.* 2022, 4, 6, 4208–4218
2. Ghorai S., Jana B., Pan D., Ramasamy T., Parshi N., Arumugam G., Ganguly J., *J Appl Polym Sci.* 2022;139:e52908
3. Parshi N, Pan D, Jana B, Ganguly J, *Sensors and Actuators: B. Chemical*, 331 (2021) 129419.
4. Maity S, Parshi N, Prodhan C, Chaudhuri K, Ganguly J. *Carbohydrate polymers*, 251, 2021, 116999.
5. Parshi N, Pan D, Dhavle V, Jana B, Maity S, Ganguly J, , *International journal of biological macromolecules*, 141, (2019), 626-35.
6. Maity S, Parshi N, Prodhan C, Chaudhuri K, Ganguly J. *Carbohydrate polymers*, 193, 2018,119-28.

B. Sc. & M. Sc.: Burdwan University [1995, 1997]
Ph.D.: Indian Institute of Chemical Biology, Jadavpur, Kolkata, India,
[Degree awarded by Jadavpur University], 2003
Specialization: Organic Chemistry.

Postdoctoral Position:

- Complex Carbohydrate Research Center (CCRC), University of Georgia,
  Athens, GA, USA (2009-2011).

Employment details:

- Associate Professor, Department of Chemistry,
  (Indian Institute of Engineering Science and Technology, Shibpur,
  (2003 to Present)
- Lecturer, Uluberia College, Calcutta University, Howrah, (2002-2003)

Awards / Honors/Membership:

1. Association Of Carbohydrate Chemists & Technologists (India) (LM)
2. Fellow of Indian Chemical Society

- Young Faculty Research Award-2015
  [BECAA – WMA And GAABESU Shibpur Foundation USA]

Current Research Interest:

- ✓ Synthesis: Sugar-based materials, Colloidal, Hydrogel, Organogel
  [Design, spectral analysis, Interaction of Supramolecular assembly]
- ✓ Glycobiology from natural resources (*Algae, mushrooms, bacteria, plant, bamboo etc.)*
- ✓ Microencapsulation of Nanoparticles and applications

Publications: 60 PhD guided: 11 ongoing: 02 PG Guided: 32 ongoing: 02

Dr. Paresh Nath Chatterjee

Making and Breaking of Carbon–Carbon Bonds in Heterogeneous Media

Dr. Paresh Nath Chatterjee
Department of Chemistry, National Institute of Technology Durgapur, Mahatma Gandhi Avenue, Durgapur 713209, Paschim Bardhaman, West Bengal INDIA
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Abstract:

In organic chemistry, many C−C bond forming methods have been developed in contrast to only a few C−C bond cleaving transformations. The challenges involved in breaking a C−C bond are known to be three-fold: thermodynamic, kinetic, and statistic. In this abstract we will highlight (i) a magnetically separable catalyst for C−C bond formation via Suzuki-Miyaura cross coupling reaction and (ii) a hypercrosslinked polymer based organocatalyst for C−C bond cleaving route. The magnetically separable heterogeneous catalyst is synthesized via a redoxdriven path from Fe3O4 and PdCl2 under modified hydrothermal technique.1 The catalyst shows excellent catalytic activity in water without the assistance of ligands, organic solvents or phase transfer catalysts. On the other hand, the hypercrosslinked polymeric catalyst is synthesized via a simple Friedel-Craft-based crosslinking reaction with tetraphenylethylene as a monomer and formaldehyde dimethylacetal as the cross linker. Sulfonation of the polymer is successfully carried out using chlorosulfonic acid. 2 This catalyst behaves like a heterogeneous Brønsted acid and catalyses a challenging dual C−C bond breaking reaction for the synthesis of symmetrical triarylmethanes (TRAMs).3 Both the catalysts are easily recoverable from the reaction media and reusable up to 5/6 cycles without significant loss in their catalytic efficacy.

References:

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Dr. Paresh Nath Chatterjee Completed B.Sc. in Chemistry honours from University of Calcutta in 2003. M.Sc. with Organic Chemistry specialization from University of Calcutta in 2005. Almost one-year post-M.Sc. industrial experience in Chembiotek Research International Pvt. Ltd., Kolkata (currently known as TCG Life Sciences). Completed PhD in the field of Organometallic & Catalysis from IIT Kharagpur in 2012 under the joint supervision of Prof. Sujit Roy (currently at IIT Bhubaneswar) and Prof. Manish Bhattacharjee. Almost one year of post-PhD teaching experience as Assistant Professor of Chemistry in Techno India, Salt Lake campus. Joined NIT Meghalaya as Assistant Professor of Chemistry in 2013 and served till August 2022 in various capacities. Presently, Dr. Chhatterjee has joined the department of chemistry, NIT Durgapur as an Associate Professor. Research domain: Catalysis in homogeneous and heterogeneous media.

An automated machine learning-based approach for estimating the air corrosion rate of low alloy steel

Usha Sharma[1]
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Abstract:

Stainless steel is an excellent material for a wide range of applications, so ensuring its durability is vital. In this research, air corrosion behavior of low alloy steel is studied in structural applications in order to develop a practical adaptive neuro-fuzzy inference system (ANFIS) for predicting atmospheric corrosion rate. These datasets are generated from the test results of air corrosion in tropical climates. The ANFIS model uses seven chemical factors that affect corrosion, namely the mean temperature, the mean moisture content, rainfall data, wetting time, the number of hours of sunlight, the average composition of chlorides ions, and the exposure of metals to air containing gases like CO2, SO2. In parallel, a suitable ANFIS model with a high coefficient of determination of 0.999 and a small root mean square error of 0.281 mg/m2 month is used to forecasts the air corrosion rate of low alloy steel. According to the sensitivity analysis, rainfall and sunlight hours have the highest impact on air corrosion rate prediction. As compared to exposure of metals to gases such as CO2, SO2, and mean temperature, the wetting times, and exposure to air containing CO2, SO2, are least severe to air corrosion rate prediction. As a final step, a graphical user interface for estimating low alloy steel air corrosion will be developed.

Anticorrosion and adsorption performance of thiazole derivative on mild steel in HCl medium

Raj Kumar Mehta, Mahendra Yadav

Department of Chemistry and Chemical Biology, Indian Institute of Technology (Indian School of Mines), Dhanbad-826004, India.

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Abstract:

The investigation shows that the corrosion inhibition and adsorption studies of thiazole derivatives namely, 2-amino-N-(benzo[d]thiazole-2-yl)-5,6-dihydro-4h-cyclopenta[*b*]thio-phene-3-carboxamide (ABTC) in 15% HCl solution for the mild steel. Weight loss and the electrochemical impedance spectroscopy technique were used to assess their beneficial inhibitory abilities. The fundamental essential aspect in the protective mechanism is the chemical and physical adsorption of inhibitors on the exposed metal surface. From, the EIS study the inhibitor ABTC had 94.6% percent inhibitory efficiency at an optimal concentration of 200 ppm (303 K). Gravimetric measurements show that at 303 K, corrosion inhibition efficiency is 95.5% at 200 ppm of inhibitor concentration. Due to the inhibitors' significant chemical and physical adsorption on the metallic substrate, the corrosion inhibition efficiency remained significantly high at increased temperatures. The tafel electrochemical investigation confirms that inhibitors reduce the both anodic and cathodic corrosion reactions.

Keywords: *Mild steel, HCl, EIS, AFM, FESEM, Quantum study.*

Modified Chitosan-based biomaterial as a suitable scaffold for bone tissue Engineering

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Abstract:

Increasing demand for artificially synthesized materials have led to rapid growth in polymeric-biomaterials market **[1]**. Incorporating certain functional groups enables them to mimic extracellular-matrix **[2]**. Chitosan is known to be excellent for tissue engineering but has poor water solubility, which can be increased by some structural modifications. Here, we synthesized a chitosan-based biomaterial modified with a monomer. It was characterized for various physico-chemical properties, such as FTIR, UV-Visible Spectroscopy, TGA, SEM etc. It was further characterized for its biological properties on bone cells i.e., on osteoblast (SaOS-2) and pre-osteoclast (RAW 264.7). The results obtained indicates successful modification of the polymer, which exhibits excellent biocompatibility for both the cell-lines. In addition, the

material show antibacterial properties against both "Gram +ve" (*S. aureus*) and "Gram -ve" (*K. pneumoniae*) bacteria. It can also be used as a drug delivery vehicle. We propose that this material can be used as a scaffold for bone mineralization for bone tissue engineering.

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A Transparent, Adhesive, Flexible and Ultra-highly Stretchable Pressure and Electro Responsive Hydrogel as Strain Sensor

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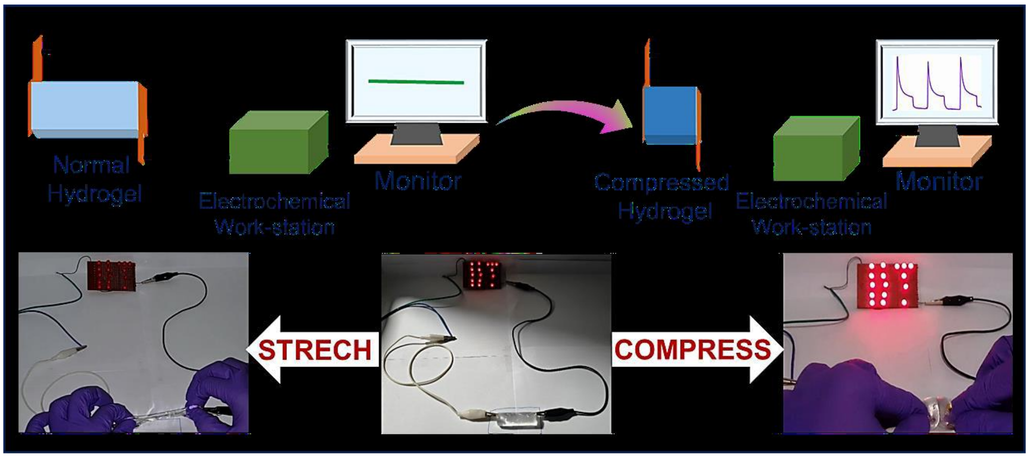
Abstract:

A multi-stimuli responsive hydrogel has been developed through the grafting of acrylamide and *N*-hydroxymethylacrylamide onto β-Cyclodextrin skeleton.[1] The hydrogel β-CD-*g*-(pAAm/pHMAm) exhibited several noteworthy features including ultra-high stretchability (>6000%), flexibility, stab resistivity, self-recoverability, electro-responsiveness, pressure-responsiveness, adhesiveness and high transparency (>90%). Additionally, the gel exhibit biocompatibility, UV resistance as well as thermoresponsive shape memory properties. Based on these striking properties of the hydrogel, a flexible transparent pressure sensor for the real time monitoring of human motion have been fabricated. Moreover, the sensor based on the gel demonstrated high sensitivity (0.051 kPa−1 for 0–3.3 kPa) due to its nanofibrillar surface morphology. The flexible sensor exhibits very rapid response time (130 ms-210 ms) with acceptable stability (5000 cycles). Remarkably, the sensor can quickly sense both robust (index finger and wrist motions) as well as the tiny (swallowing, phonation) physiological actions.



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Role of chemicals for prevention and control of coal mine fires and explosions

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Abstract:
Coal mine fires and explosions are a severe issue for the safety of coal miners and mines. This paper presents the role of chemicals in the prevention and control of coal mine fires and explosions. A coal mine fire occurs mainly due to a slow oxidation process, i.e., spontaneous heating of coal, whereas a coal dust/gas explosion is a sudden outburst of combustible fuels either triggered by the spontaneous heating/fire of coal or other external heat energy in mines. So, different heating rates play an important role in the study of spontaneous heating/fire/explosion of coal in the laboratory. The differential scanning calorimeter (DSC) technique was used to explore the thermal behaviour of some chemicals at slow and high heating rates. Results revealed that chemicals have various endothermic and exothermic energies at different heating rates. It was concluded that different chemicals (either single or combinations) may be used for the prevention and control of coal mine fires and explosions for the safety of coal miners, mines, and the environment.

Keywords: Coal, chemicals, spontaneous heating, fire, explosion.

Multicolour Emissive N-doped Carbon Quantum Dots for FRET Dissection of Gold Nanorods

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Abstract:

Gold nanorods (AuNRs) have become some of the most used nanostructures for biosensing and imaging applications due to their plasmon-related optical response. Owing to aspect ratio, gold nanorods (AuNRs) showed short wavelength transverse and long wavelength longitudinal absorption. The FRET between carbon quantum dots (CQDs) and AuNRs may arise from distinctive overlap of transverse and longitudinal bands of AuNRs with fluorescence (FL) spectra of CQDs. In this context, we have developed a fluorometric probe for the detection of glucose, glutathione and acetylcholinestrase enzyme. A series of Nitrogen-doped carbon quantum dots (Blue, Green, Orange and Red) were synthesized by hydrothermal method. The fluorescence resonance energy transfer (FRET) based fluorescence "switch-off-on" of N-CQDs (energy donor) in presence of gold nanorods (energy acceptor) has been successfully applied to fabricate a fluorometric probe for the detection purpose. The interruption of the FRET phenomenon by the production of H2O2 and thiol group from the reaction of glucose oxidase in presence of glucose, and glutathione as well as acetylcholinesterase (AChE) enzyme respectively causes the FL recovery of N-CQDs.

KEYWORDS: N-CQDs, AuNRs, glucose oxidase, glutathione, acetylcholinesterase

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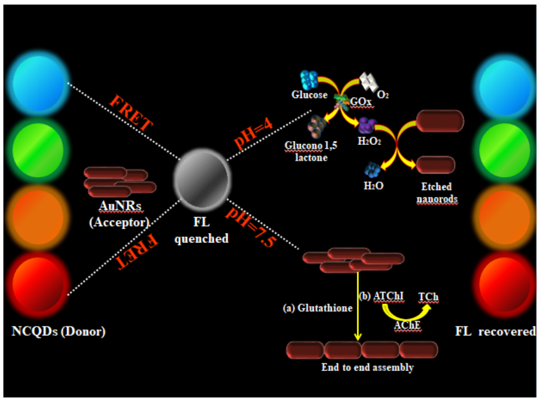

Polyaromatic hydrocarbons based synthetic heat transfer fluid: Synthesis and stability studies

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Abstract:

Thermal fluids are also known as heat transfer fluid. Thermal fluids are used in heating systems which operate in a closed-loop. Synthetic heat transfer fluids deliver efficient, dependable and uniform heat at very low pressure. These fluids are best specified where natural fluids cannot work at system temperatures more than 320°C and its posse's low vapor pressure. Because of its low vapour pressure synthetic aromatic heat transfer fluids are used in solar applications worldwide. Concentrating solar power (CSP) are having inherent energy storage because of the heat carrying capacity of the thermal fluid and which allows the system to operate during periods of low or absence solar irradiance. Commonly used thermal fluids are biphenyl oxides but these fluids are not functioning above 400°C operating temperatures, which is less than ideal for most power-generation steam turbines and solar systems. Thus, a heat transfer fluid having stability >400°C is highly desired. Polyaromatic phenyl naphthalene-based molecules are such type of organic molecules which are known to have stability at higher temperature.

We have developed organic heat transfer fluid based on polyaromatic phenyl naphthalene molecules. These molecules were prepared by an environmentally benign synthetic methodology using refinery spent catalyst. Thermal stability studies of phenyl naphthalene based thermal fluid were carried out at different temperatures using suitable radical scavenger and found stable up to 450°C. Details about the catalytic activity and thermal stability of developed thermal fluid will be discussed in the research paper.

KEYWORDS: Heat transfer fluids, phenyl naphthalene, polyaromatic, thermal stability

Production of Biosurfactant from Microorganism

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Abstract:

Biosurfactants are active compounds that are produced at the microbial cell surface or extracted from microorganism. Biosurfactants are potentially replacements for synthetic surfactants in several industrial processes such as lubrication, wetting, softening as well as in food, biomedical and pharmaceutical industry.1-3 Biosurfactants have advantages compared to chemical surfactants in heaving lower toxicity, higher biodegradability, pH levels and abilities to be synthesized from renewable feed stocks. Very often the growth of microorganisms on hydrocarbons is accompanied by the production of emulsifying's agents that causes emulsification of hydrocarbon sources in the culture medium.4 Three microbial strains have been used for the production of biosurfactants *Rhizopus Nigrican*- SB12, S1(tentatively *Fusarium)* and A1 (unidenfied). The microbial lipid collected from theses microorganism have shown surface properties. The interfacial tension of the chloroform solution of these lipids are 17.3 mN/m (*Rhizopus Nigrican*- SB12); 13.6 mN/m (A1) and 18.4 mN/m (S1 *Fusarium*) and the critical micelle concentrations (CMC) of these microbial lipids are 2.5gm/Lit, 1.9 gm/Lit and 1.0 gm/Lit respectively.

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Sustainable Aviation Fuel and ASTM D2425: Analysis of Hydrocarbon Types and Its Limitation

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Abstract:

In line with various other sectors, aviation sector has also undertaken net-zero emission targets for CO_2 by 2050. Application of sustainable aviation fuel (SAF) alongside petroleum origin aviation turbine fuel (ATF) is proposed to be a game changer in achieving the said target. Limits for aromatics and cycloparaffin content in ATF is prescribed by ASTM D7566 specifications. As per specification, ASTM D2425 is the recommended method for hydrocarbon composition in SAF. However, application of D2425, which is originally meant for petroleum middle distillates, with significant aromatics and less of isoparaffins, has serious drawbacks with SAF, a synthetic product of relatively lighter nature and having very low aromatics and high isoparaffins. It has been observed that the amount of cycloparaffins, a compliance parameter, comes in significantly higher side while SAF is estimated following ASTM D2425 method. It was noticed that presence of higher amount of isoparaffins in a sample led to higher estimation for cylcoparaffins by D2425. In order to understand the intricacies of the analysis, two samples of SAF and few known synthetic blends were analyzed by NMR, GC-MS and ASTM D2425. Results of this study including comparison of quantitative data and qualitative analysis will be presented.

Keywords: SAF, ASTM D2425, NMR, Mass.

$MoSn_2Se_4$-decorated MXene/Functionalized-RGO nanohybrid for ultrastable Supercapacitor and Oxygen Evolution Catalyst

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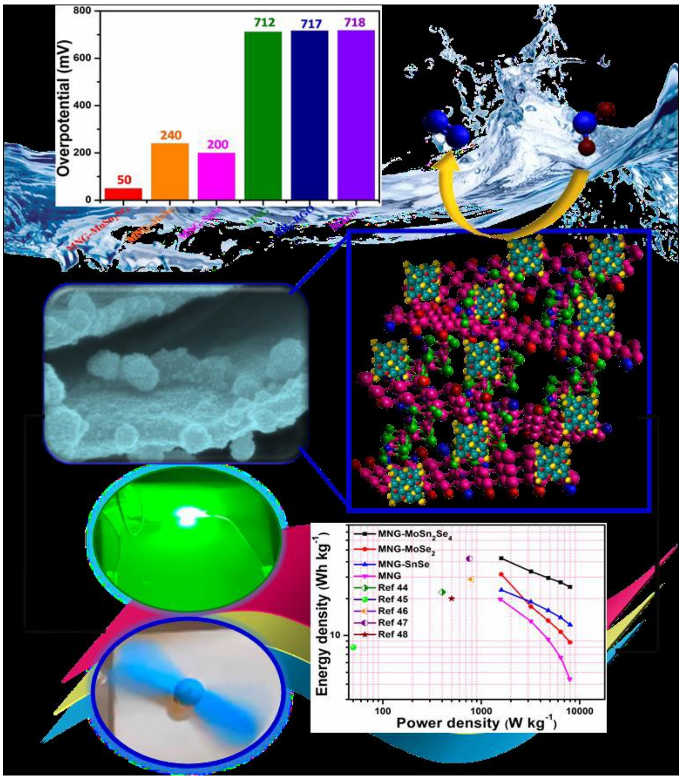
Abstract:

In this study, Mo and/or Sn selenides were grown on a template of Ti3C2Tx/NH2-RGO binary composite material via facile hydrothermal method. Superior electrocatalytic activity was obtained from $Ti_3C_2T_x/NH_2$-RGO/$MoSn_2Se_4$ electrocatalyst with an onset potential of 1.3 V (vs. RHE), lower overpotential (□10) of 50 mV, large electrochemically active surface area, and smaller Tafel slope of 55.9 mV dec-1 with durable electrocatalytic performance. The assembled asymmetric supercapacitor device using our synthesized material as cathode showed excellent performance with high specific capacitance (120.2 F g−1), large energy density (42.7 W h kg−1), and ultrastability with 97 % capacitance retention after 10000 charging-discharging cycles. This work provides an overall insight into designing an electrode material for both efficient oxygen evolution as well as high performance supercapacitor device.



Structural investigation of Zn-MoF for Hydrogen storage application

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Abstract:

Metal organic frameworks (MOFs) have gained many popularities in gas storage in last two decades and possess an organic flexible scaffold, furnishing a porous structure with large surface area which is inevitable for gas storage.

We report novel Zn (II)-based metal organic frameworks (Zn-L1L2) based on mixed organic ligands of 1,3,5-benzene tricarboxylic acid (BTC) (L1) and 2-methylimidazole (mIm) (L2) stemming from solvothermal-mediated synthesis. Zn-L1L2 was characterized using various analytical techniques such as single-crystal X-ray diffraction (SC-XRD), transmission electron microscopy (TEM), X-ray photo electron spectroscopy (XPS). ZnL1L2 crystallizes into polymorphs in tetragonal system with space group I41/a. It has an infinite three-dimensional architecture with three crystallographically independent Zn atoms bridged by oxygen atom of carboxylic acid of BTC and nitrogen atoms of MIM in the symmetric unit. The C-O distances of Carboxylic acid and the C-N bond distances of imidazole unit are within the ranges reported in the literature. The sample exhibited rods like morphology in 2D form and the EDX confirms the presence of Zn, C, N, O elements in the sample. Moreover, STEM mapping of the particle shows the uniform distribution of main elements of zinc, nitrogen and oxygen. The synthesized material was further characterized by XPS to understand the chemical state. The C1s peak is largely fitted with sp^3 (~284.3 eV), sp^2 (~285.3 eV) and C-N (~285.8 eV) groups in addition to a $\pi - \pi^*$ (291.6 eV) shakeup structure. The N1s shows the signals at 398.0 eV for N-C, 399.2 eV for N-H, and 401.5 eV for N-Zn. The hydrogen adsorption capability of the ZnL1L2 is evaluated at room temperature and is found to be in the range of 0.92 to 1.5wt%.

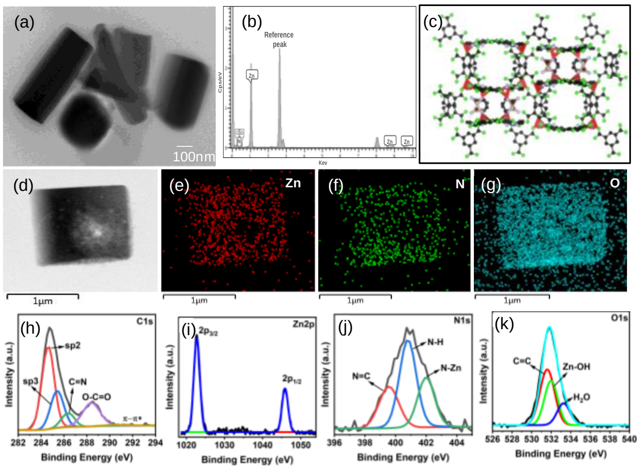

Fig.1. (a) TEM image of ZnL1L2, (b) EDS spectrum of ZNL1L2, (c) Single crystal-XRD ZNL1L2, (d, e, f, g) STEM mapping of ZnL1L2 and (h, I, j, k) XRS spectra of Z

A Smart Polyester Synthesised from Polyol and Tri-Acid Tethering Bio-Application

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Abstract:

A smart polyester with branched /hyperbranched architecture was synthesised from condensation polymerisation between a polyol and a tri-acid with varied stoichiometry for promoting bio application. An increase in tri acid content increased the extent of branching alongside increased the extent of cross linking, simultaneously. The micro-structure of the branched polyesters was established through spectroscopy, viscometry, and morphological findings. The sample having optimal level of branching and cross linking possessed enough microscopic voids which promoted adhesion and growth of eukaryotic cells due to supply of adequate food and nutrients from the biocompatible polyester matrix. Alongside, inhibitory, and growth-promoting actions both have been observed with prokaryotic cells simultaneously leveraging antimicrobial as well as growth media supplementation properties by some of these polyesters as well.

Keywords: Branching, Polyol, Tri-acid, Bio-application

Graphene oxide supported *N*-heterocyclic carbene copper(I) complex for selective *N*-monoalkylation of amines *via* hydrogen auto-transfer strategy

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Abstract:

In recent years, *N*-heterocyclic carbenes (NHCs) transition metal complexes have been used as both homo- and heterogeneous catalysts in several organic transformations with spectacular success.1,2 The superiority of NHCs ligands over plethora of other ligands is ascribed to the better σ-donating properties and steric hindrance of NHC ligands.3 However, only a few examples of NHC ligands, covalently linked to the surface of graphene oxide (GO), are reported to date.4,5 In this manuscript, we describe the synthesis and characterization of a new *N*-heterocyclic carbene copper(I) complex supported on graphene oxide (GO-NHC-Cu). The catalytic activity of the supported complex was explored in *N*-alkylation of anilines with alcohols under solvent-free and aerobic conditions to afford the monoalkylated products in good to excellent yields. All the products were isolated and characterised by NMR spectroscopy. The catalyst can be easily recuperated and reused for up to five consecutive cycles with insignificant loss in the catalytic activity.

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Development of cucurbit[6]uril supported *β*-Ni(OH)2 nanoparticles for quinazolines synthesis *via* acceptorless dehydrogenative coupling

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Abstract:

Nitrogen containing heterocyclic compounds such as quinazolines occupy a core structure in various biologically active compounds which are used as commercialized drugs.1,2 Therefore, there is a pursuit for the development of efficient, green, atom economic methods using readily available and inexpensive starting materials for the synthesis of quinazolines.3-5 In this perspective a cucurbit[6]uril supported *β*-Ni(OH)2 nanoparticles, *β*-Ni(OH)2-CB[6], was designed and characterized using several physicochemical techniques. The nanocomposite was successfully applied as a heterogeneous catalyst in the synthesis of quinazolines, in excellent yields and high turnover numbers (TON), *via* acceptor less dehydrogenative coupling (ADC) of alcohols with nitriles. The nano catalyst was found to be an efficient and robust catalyst that can be reused up to four times with negligible loss in catalytic activity. The reaction protocol was found to be atom-economical and sustainable. The research paves the way for the development of prodigious and sustainable heterogeneous catalysts in future.

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Photocatalytic CO_2 to Methanol Conversion by g-CNQDs@MOF Composite under Visible Light Irradiation

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Abstract:

Considering the global warming due to accumulation of excess CO_2 in the atmosphere, it is vital to reduce the CO_2 emissions by capturing or converting it into value-added chemicals and fuels. Among the known materials, MOFs have great significance in capturing the CO_2 and its conversion into energy efficient fuels due to their inherent chemical, physical and optical properties. In this study, graphitic carbon nitride quantum dots coupled Zr (IV) based MOF composite (g-CNQDs@MOF) has been reported for the photoreduction of CO_2 to methanol selectively under visible light irradiation. g-CNQDs in the Zr-based MOF composite play important role for photocatalytic CO_2 reduction due to its electron availability, thereby improving the electronic conductance properties of the composite. The synergistic effect of the composite enhances the charge separation and generates many catalytically active sites on the MOF's surface to reduce CO_2 selectively into methanol with better selectivity and efficient methanol formation rate.

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A Rational Design of Multicolor Emissive Carbon Dots for Efficient White-Light-Emitting Diodes and Room-Temperature Phosphorescence

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Abstract:

Multicolor tuning is one of the most remarkable features of carbon dots (CDs), used as a color convertor in making white-light-emitting diodes (WLEDs). [1,2] Herein, a solvent-controlled method has employed to prepare the multicolor emissive CDs from 1, 2, 4-triaminobenzene and melamine, where the G-, O-, and R-CDs have been synthesized in different solvent. To avoid the aggregation quenching emission (AQE), fluorescent polymeric films have shaped by mixing PMMA with R- and G-CDs, while O-CDs made with PVA. Interestingly, PVA exhibited red-shifted emission of O-CDs from 585 to 597 nm in O-CDs/PVA, while PMMA accompanied a blue-shifting emission. The fluorescent solid films have used to develop monochromatic and white-color emissive LEDs. Further, all the synthesized CDs served as a carbon precursor to develop room-temperature phosphorescence (RTP) by molten salt method, where only R- and O-CDs achieve their RTP emissions with different intensities. The mechanism behind the RTP formation with CDs and their emission intensity dependency has studied by the C=O moieties.

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Synthesis and Characterization of Copper-triazine-dendrimer functionalized graphene oxide (GTD-Cu): Application in green synthesis of propargylamines

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Abstract:

A^3 -couplings are one of the most exploited multicomponent reactions for the synthesis of propargylamines due to one-pot simple experimental procedure and inexpensive reactants.[1] Numerous propargylamine derivatives are integral part of the core structure of many pharmaceutically active compounds.[2] So, the development of new protocols for the synthesis of such types of molecules is an emerging area of research. Dendrimers are a new class of polymeric materials showing high density of surface functional groups, repetitive and symmetrical branched structures and may serve as ideal scaffolds for the encapsulation of various transition metal ions.[3] In this perspective, a copper-triazine-dendrimer functionalized graphene oxide complex (GTD-Cu) was synthesized and characterized by various physico-chemical techniques. The synthesized complex was found to be a good heterogeneous catalyst for the synthesis of a series of propargylamines via A^3 -coupling reaction in an aqueous medium (Figure 1).

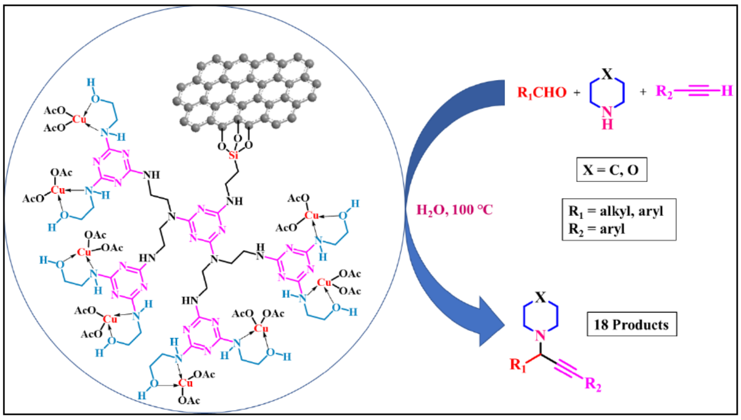

Figure 1: Synthesis of propargylamines

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The magical metalloporphyrins: Mirror, Mirror on the Wall; Which is the Best Porphyrin of them all?

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Abstract:

The sterically protected and electronically activated metalloporphyrins find myriad applications from drug metabolism, valorisation of biomass, production of fine chemicals and environmental remediation. We report herein an entirely recent activity and potential utility in flame retardancy of polyurethanes. Catalytic oxidation by aza-macrocycles was investigated by us for potential use as flame retardants in polymers. Substituted tetraphenyl porphyrins with transition metal centers were used in polyurethane systems to catalyse the formation of a protective layer of char to attenuate and improve flame retardancy. The comparative analysis of increased catalytic activity of various substituted tetraphenyl porphyrins was another key component of this work. We have also explored other diversely substituted azamacrocycles and drawn correlations between activity and composition of the core.

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An Amino Acid Inspired Fluorescent Copolymer via RAFT Polymerization with concentration dependent Cube and Rod like self-Aggregation

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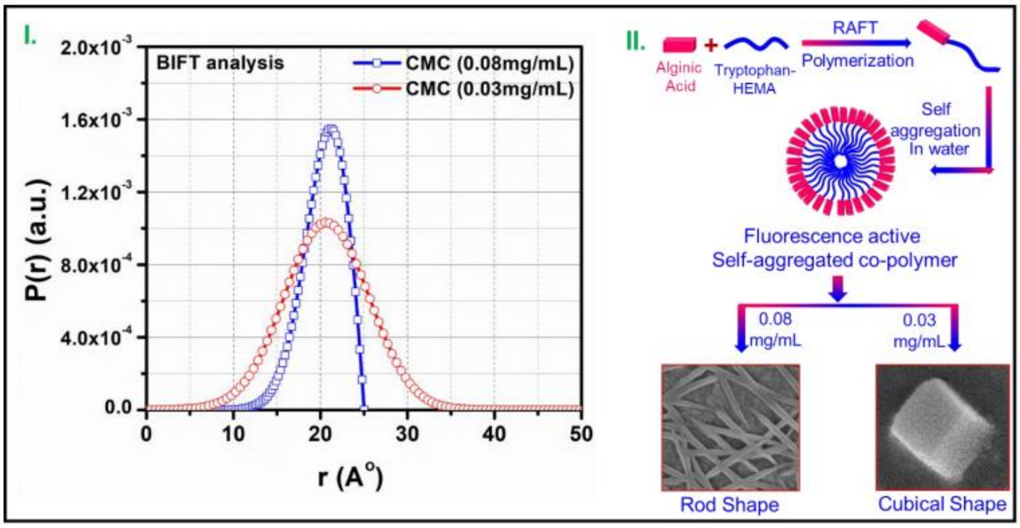
Abstract:

A hydrophobic monomer N-Boc tryptophan-hydroxy methyl methacrylate (HBT) has been synthesized by chemical modification of N-Boc tryptophan. This monomer has further been grafted through RAFT polymerization on the backbone of raft reagent modified alginic acid to obtain a new fluorescent amphiphilic copolymer with attached hydrophobic segment. The controlled polymerization is assessed using Advanced Polymer Chromatography with a narrow distribution. The critical aggregation concentration of the developed copolymer has been determined by surface tension, photoluminescence spectroscopic and dynamic light scattering analyses. The size and shape of the developed micelle has been investigated by FESEM and HRTEM analyses, which revels concentration dependent change in morphology through self-aggregation. The existence of rod and cubic shape in two different concentrations has also been verified by small angle X-ray scattering (SAXS). The formed self-aggregation is able to uptake and release a model hydrophobic drug (naproxen) in controlled manner in different rate in two different concentrations.



A Supramolecular Tb(III)- metallogel with Admirable Charge Transport Properties

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Abstract:

Gels are the gift of serendipity.[1] Supramolecular gel[2] formation is the most exciting result of supramolecular self-assembly,[3] ceaselessly strengthening materials science through various applications. Molecular self-assembly is the vital responsible factor for the development of supramolecular metallogel. During the gel materialization, the solvent molecules are immobilized in a three-dimensional (3D) supramolecular network of gelator molecules, and the gel formation can be primarily identified by an inversion-vial test.[1]

Here, we have synthesised a terbium(III)-ion-based supramolecular metallogel with oxalic acid dihydrate as a potential low-molecularweight organic gel-forming constituent in N,N-dimethylformamide (DMF) solvent under ambient conditions.[4] In-depth studies and analyses of the optical and electrical parameters of Tb(III)- metallogel establish the semiconducting properties of the Tb(III)- metallogel. Based on its conducting properties, the Tb(III)- metallogel is effectively applied to a metal-semiconductor junction-based photosensitive Schottky barrier diode device with admirable charge transport properties.

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A pilot scale demonstration of $O_3/H_2O_2/UV$ coupled solar concentrator with membrane bioreactor and activated carbon for treatment of petrochemical wastewater

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Abstract:

In this investigation, a 1000 L pilot plant was developed to treat ethylene glycol (EG)-laden petrochemical wastewater through advanced oxidation processes (AOPs) coupled membrane bioreactor and activated carbon (MBR-AC) (Fig.1). At an optimum operating condition (H_2O_2 of 5 mM, ozone dosage of 1 mg/L, and UV fluence of 45 W/m^2), 93% degradation of 750 mg/L of EG and 55% removal of total organic carbon (TOC) were achieved by $O_3/H_2O_2/UV$ after 110 min. However, only 31%, 22.5%, 14.2%, 7%, 4%, and 1.2% of TOC and 70.5%, 61.7%, 48.2%, 40.4%, 30%, and 14.8% degradation of EG were observed by O_3/UV, O_3/H_2O_2, UV/H_2O_2, O_3, UV, and solar processes, respectively. Moreover, ~100% degradation of EG and 75% mineralization was observed by AOPs coupled MBR-AC system. The electrical energy per order and total operating cost of treating per m^3 of EG by AOPs coupled MBR-AC was observed to be 1.067 kWh m^{-3} $order^{-1}$ and 0.27 \$ m^{-3} $order^{-1}$, respectively.

Keywords: Advanced oxidation processes; Ethylene glycol; Membrane Bio-reactor; Petrochemical wastewater treatment; Solar concentrator reactor

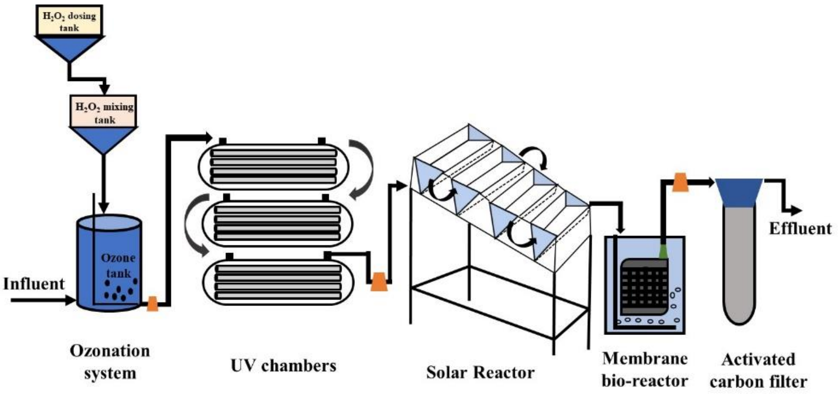

Fig. 1: Schematic of AOPs coupled MBR-AC syste

Facile synthesis of CDs deposited *γ*-FeOOH nanosheet/Polypyrrole composite: a promising photocatalyst for degradation of antibiotic under sunlight

*Abanindra Nath Sarkar and Sagar Pal**

Abstract:

A facile in-situ approach was employed to fabricate a ternary nanocomposite using exfoliated *γ*-FeOOH, carbon dots (CDs) and polypyrrole in a single pot along with its application as a photocatalyst towards degradation of antibiotic under sunlight. Here, the expired pharmaceutical drugs (waste) were used as a source of CDs synthesis to meet the Waste-to-Wealth approach. Amongst all prepared composites including binary and trinary nanocomposites, the excellent photocatalytic activity of PFL/CDs-2 can be attributed to synergistic enhancement of the light harvesting of *γ*-FeOOH nanosheet and the inhibited recombination rate of photoexcited charge carriers based on a Z-scheme photocatalytic mechanism. Besides, antibacterial potential of synthesized composites was studied against *Bacillus pumilus* (Gram-positive) and *Escherichia coli* (Gram-negative) bacteria. Moreover, PFL/CDs-2 composite was found to be magnetically separable and recycled without a significant loss of photocatalytic efficiency after four cycles, indicating the high reusability and stability of the photocatalyst.

Influence of phase boundary on magnetic and magnetocaloric properties of nanocrystalline $La_{0.17}Ca_{0.83}MnO_3$ sample

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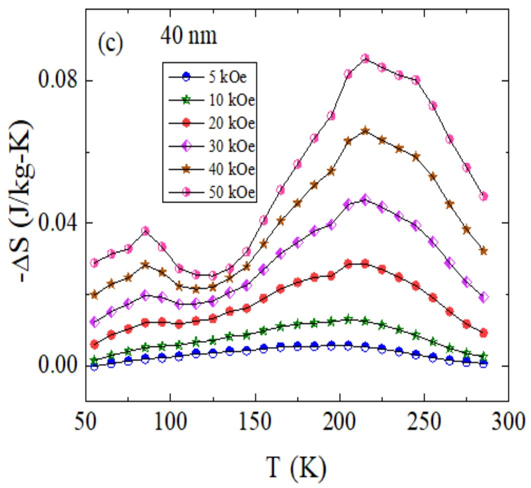
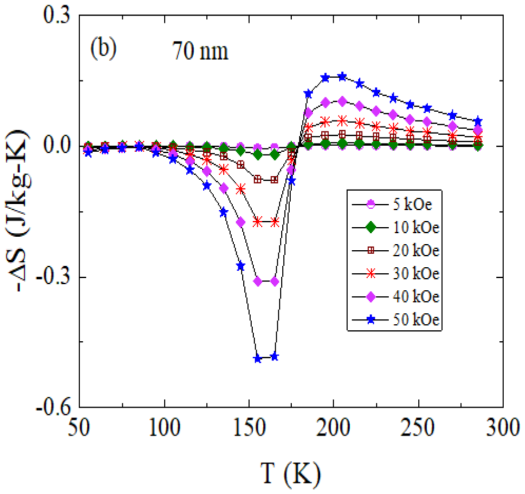
Abstract

In this present study we report the Magnetic properties and magnetocaloric effect of two nanocrystalline $La_{0.17}Ca_{0.83}MnO_3$ samples prepared by sol-gel method with average particle size ~40 nm and ~70 nm. The characterization of the samples is done by Rietveld refinement using PXRD data and we have also reported the structure, particle size and chemical composition by SEM and EDX. The above-mentioned studies reveal that samples are single phase mixed perovskite nanoparticles of 'pnma' space group. According to the reported phase diagram, the bulk compound lies near the phase boundary between charge ordered antiferromagnetic and canted antiferromagnetic state. In contrast to the bulk counterpart, the significant effect of the phase boundary was observed on the physical properties of nanocrystalline compounds. Moreover, the signature of canted magnetic phase in nanocrystalline sample was probed through magnetocaloric effect study.





Selective hydroxylation of benzene to phenol via C-H activation over mesoporous Fe_2O_3-TiO_2 using H_2O_2

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Abstract:

The omnipresence of C-H bonds in organic molecules enamors chemists for the functionalization of C-H bonds towards value-added molecular scaffolds.1 Mesoporous Fe2O3-TiO2 mix-oxide catalyst has been successfully synthesized via a triblock-copolymer (P123) mediated sol-gel method and catalytically tested in selective hydroxylation of benzene. The physicochemical characterizations evidence that Fe(III) ions incorporate into the pure anatase TiO2 lattice framework. The presence of surface protons was determined by the TPD analysis. The NH3-TPD results show that the 5 wt% Fe-TiO2 has a higher total acidity of 105 μmol/g. Interestingly, a further increase in iron amount decreases the total acidity. The surface protons were counterbalanced by the negative charge in the crystal lattice of TiO2, which originated due to the substitution of Ti4+ by Fe3+.2 Herein, we observe that the surface acidity directs the selectivity towards phenol. Under the optimized conditions, 5% Fe-TiO2 with notified strong acid sites gives a higher phenol yield of 31.2 % with > 99 % selectivity; moreover, the catalyst is reusable at least four times.3

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Zeolite-Na-Y entrapped Cobalt Acyl pyrazolone complexes as heterogeneous catalysts for catalytic Styrene oxidation reaction

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Abstract:

Transition metal cobalt Acyl pyrazolone complex $[Co(L_3)_2(H_2O)_2]$ has been prepared by β-diketone interaction of Acyl pyrazolone ligand 4-(4-chlorobenzoyl)-5-methyl-2-(p-tolyl)- 1,2-dihydro-3H-pyrazol-3-one with $CoCl_2.6H_2O$. The complex is characterized by FTIR, TGA, Mass spectrometry and XRD. Cobalt complexes have been entrapped in zeolite Na-Y by flexible ligand method. Synthesized materials have been characterized by FTIR, TGA and GC. zeolite Na-Y entrapped transition metal complexes was examined in oxidation of styrene using 30% H_2O_2 as an oxidant beside neat complexes to check the aptitude of heterogeneous catalysis over the homogeneous system. The effect of experimental variables such as mole ratio of substrate to an oxidant, amount of catalyst, reaction time, varying oxidants, and solvents on the conversion of styrene was also tested. one of the zeolite Na-Y entrapped transition metal complex viz. $[Co(L_3)_2(H_2O)_2]$-Y was found to be a potential contender for styrene oxidation reaction.

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$BaBi_2Nb_2O_9$ layered structured nanoceramics for energy storage application, fatigue-free relaxor ferroelectric behaviour

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Abstract:

Ferroelectric ceramics with lead-free bismuth layers are crucial for advanced energy storage applications. A wide range of applications are anticipated for the thin hysteresis curve with excellent energy storage density and efficiency. The current study uses 5% yttrium instead of bismuth in $BaBi_2Nb_2O_9$ relaxor ferroelectrics to investigate the aforementioned objectives. The diffused phase transition and extensive temperature dependency of the dielectric properties revealed the material's space charge polarisation as a result of the presence of Y^{3+} at various domains. The greater degree of diffuseness and low dielectric loss suggest that charge carriers had a key impact in the dielectric study's analysis of frequency and temperature variation. The material exhibits non-Debye type relaxation and NTCR behaviour, which are related to the various relaxation processes, according to impedance spectroscopy investigation. The material's suitability for usage in a future NVRAM application is demonstrated by the materials' low P-E hysteresis curve and fatigue-free characteristics up to 10^6 cycles.

Keywords: Relaxor ferroelectrics; Nanomaterials; Solid-state synthesis; Slim hysteresis; $BaBi_2Nb_2O_9$

Abstract No – D16

Modified Alginate based Polymeric Micelles via RAFT Polymerization for pH Triggered Release of Indomethacin Drug

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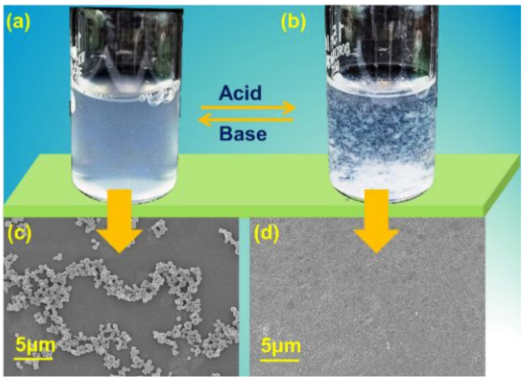
Abstract:

Reversible pH responsive biopolymeric micelles have been prepared by the self-assembly of amphiphilic Alg-g-p(Gly-HEMA) copolymer for drug-delivery of hydrophobic drug (indomethacin). Herein, a hydrophobic monomer N-Boc glycine-hydroxy methyl methacrylate (Gly-HEMA) has been synthesized by chemical modification of N-Boc glycine. This monomer has further been grafted through RAFT polymerization on the backbone of raft reagent modified alginic acid to obtain a new amphiphilic copolymer with attached hydrophobic segment. The controlled polymerization is assessed using Advanced Polymer Chromatographic (APC) analysis with a narrow distribution. The critical micelle concentration (CMC) of the developed copolymer has been determined by surface tension, photoluminescence spectroscopic (PL) and dynamic light scattering (DLS) analyses. The size and shape of the developed micelle has been investigated by FESEM and HRTEM analyses, which reveal that the size of the copolymeric micelle is ~ 200 nm with spherical in shape. Alg-g-p(Gly-HEMA) has demonstrated pH-responsive reversible micellization behaviour. The process of micellization to phase separation and vice versa can be controlled just by altering the pH. The formed micelle is able to uptake and release a model hydrophobic drug (indomethacin) in controlled manner.



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N-Doped Carbon Quantum Dot-MnO2 Nanowire FRET-based fluorescence probe for detection of cholesterol

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Abstract:

Nitrogen-doped carbon quantum dots were synthesized using the hydrothermal method. Citric acid and triethylamine were taken as precursors. The fluorescence resonance energy transfer (FRET) based fluorescence "switch off-on" of N-CQD(energy donor) in presence of MnO2 Nanowires (energy acceptor) has been successfully applied to fabricate a fluorometric probe for the detection of Cholesterol. MnO2 nanowires (MnO2 NWs) significantly quenched the blue fluorescent emission of N-CQDs by the phenomenon of FRET. The redox reactions of MnO2 with H2O2 resulted in the decomposition of MnO2 nanowires (brown) to give Mn2+ ions (colorless), which induced the fluorescence recovery of N-CQDs. The interruption of the FRET phenomenon of N-CQD-MnO2 NW composites by the produced H2O2 from the reaction of Cholesterol oxidase in the presence of cholesterol causes FL recovery of N-CQDs.

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Blue Emissive Silicon Quantum Dots as a Fluorescence Probe for the Detection of Hg2+ Ions and L-Cysteine

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Abstract:

Detection of mercury is necessary to protect environment and human health due to its high toxicity. In the present work, blue fluorescent silicon quantum dots (SiQDs) were synthesized by hydrothermal method using (3-aminopropyl)triethtoxysilane (APTES) as silicon source and trisodium citrate as a capping agent . As synthesized SiQDs were used as fluorescent probe for the detection of mercuric ion (Hg_{2+} ions) and L-Cysteine. The fluorescence of the SiQDs was turn-off when mercury is added into it and the mechanism behind this phenomenon is static fluorescence quenching of SiQDs in the presence of Hg_{2+} ions. Further, the FL intensity of SiQDs gets recovered with the addition of L-Cysteine. This is due to the Hard-Soft acid base interaction between soft acid Hg_{2+} and sulphur containing thiol group which is present in the L-Cysteine is soft base. Utilizing the fluorescence turn-off and turn-on system, the probe is applied for the detection of Hg_{2+} ions and L-Cysteine in real samples with a detection limit in µM to nM range.

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Customized Gas Chromatograph: A New Solution for LPG Analysis

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Abstract:

Analysis of hydrocarbon composition and impurities in LPG is a recurring challenge and requirement in petroleum refining and petrochemical industry. Necessary Gas Chromatograph (GC) with advanced configuration has been designed in consultation with OEM and method has been developed for estimation of hydrocarbon composition and impurities from ppm to percentage level.

Estimation of hydrocarbon composition and impurities is very important as LPG is used as feedstock for propylene, ethylene etc. Estimation of trace level permanent gases such as O2, N2, CO, CO2, H2S and other catalytic poisons namely Acetylene, Methyl Acetylene, Propadiene, Phosphine, Arsine, Carbonyl sulphide (COS) in ethylene/propylene are important because these impurities affect the production of polymers, polymer properties and characteristics, even at the ppm or ppb level. Additionally, they can also irreversibly poison the catalyst.

Two capillary column chromatographic systems equipped with an injector and two column switching valve has been used for the stated applications.

Keywords: LPG, Gas chromatograph configuration, Estimation, Hydrocarbon composition, impurities.

Synthesis and Optical study of Zn_2SiO_4: Dy^{3+} Phosphor

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Abstract:

By using solid-state reaction method, we have synthesized Zn_2SiO_4: xDy^{3+} ($x = 1, 2, 4, 6, 8,$ & 10 mol %) phosphor at 800°C. This work evaluates its properties for possible application in solid state lighting, display device etc. Synthesized phosphors were characterized by using Powder X- ray diffraction (PXRD) and crystalline size was calculated using Debye Scherer formula which was approximately ~30nm. Field emission scanning electron microscopy (FESEM) was used to investigate the morphology and structure of phosphor. Photoluminescence (PL) properties were also investigated for excitation and emission peaks of synthesized phosphor. The excitation spectra appeared at 337nm with the sharp line due to the transition from $\mathbf{{}^6H_{15/2} \rightarrow {}^4F_{15/2}}$**.** The intense emission spectra were observed at ~464 nm, 488, nm 579nm, due to $\mathbf{{}^4H_{15/2} \rightarrow {}^6I_{15/2}}$, $\mathbf{{}^4F_{9/2} \rightarrow {}^6H_{15/2}}$, $\mathbf{{}^4H_{9/2} \rightarrow {}^6H_{13/2}}$ of Zn_2SiO_4:4mol% Dy^{3+}. The Thermoluminescence(TL) and glow curve properties of synthesized Zn_2SiO_4: Dy^{3+} phosphor were studied using UV radiation, exposure time ranging from 5 min to 30 min. Through the TL glow peaks we determine the kinetic parameters such as order of kinetics (b), activation energy(E), and frequency factor(s), etc. All the Kinetic parameters of the TL glow curve are analysed by using Chen's peak shape method and initial rise method.

Keywords: Zinc Silicate, Photoluminescence, Thermoluminescence, Morphology of Crystal

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Palladium anchored N-Heterocyclic Carbene on a Porous Polymer – An Efficient Heterogeneous Composite Catalyst for Eco-Friendly Suzuki-Miyaura Coupling

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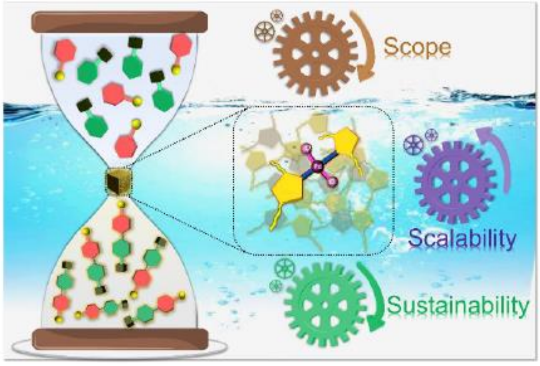
Abstract:

Aggregation induced catalyst deactivation during the reaction prevail as one of the pitfalls in supported metal catalysts.[1] Herein, homogeneously dispersed palladium coordinated N-Heterocyclic carbene was strategically integrated inside a microporous hyper-cross-linked polymer (HCP) via post-synthesis structural modulation. Successful immobilization of spatially isolated Pd (II) units onto the polymer scaffold yielded highly robust heterogeneous catalysts 120-MI@Pd NHC & 120-EI@Pd NHC, respectively. 120-EI@NHC Pd (4.41 wt% Pd loading) illustrated remarkable catalytic potency (yield up to >99%) toward eco-friendly Suzuki-Miyaura coupling (SMC) reaction at room temperature. The catalytic efficiency of 120-EI@Pd NHC is highlighted from its excellent functionality tolerance over 42 substrates and TOF value reaching up to 4.97×103 h-1. Pertaining to heterogenization, the polymer catalyst could be reused with intact catalytic efficiency for at least 10 cycles. The competence of 120-EI@NHC Pd in terms of scope, scalability and sustainability advocates its proficiency while processability was achieved with 3D aerogel monolith.[2]



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Multifunctional nitrogen rich porous organic polymer for high pressure CO2 uptake and an excellent organocatalyst for CO2 fixation reaction

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Abstract:

Global warming and climate change are two serious environmental threats brought on by the atmosphere's steadily rising carbon dioxide (CO2) concentration. Therefore, finding an appropriate sorbent as well as organocatalyst for high CO2 capture and utilization is a solution of this problem. In this context, divinylbenzene, triallylamine, and 2,4,6-tris(allyloxy)-1,3,5 triazine have been radical polymerized to create a new porous cross-linked organic polymer called DAT-1 has a high degree of flexibility, a BET surface area that is unusually large (1105 m2g-1), and bimodal porosity. Furthermore, the DAT-1 porous architecture, which is very rich in basic N-sites, combined with the triazine unit and tertiary amine moieties could make it an excellent adsorbent for the unprecedented CO2 capture (73.3 mmol g-1 30 bar/273 K). Additionally, by using carbon dioxide as a C1 resource, it exhibits excellent catalytic activity for the conversion of simple terminal epoxides to bio-derived satirically hindered epoxides to cyclic carbonate.

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Prof. Pradeepta K. Panda

Porphycene – An Emerging Isomeric Porphyrin Dye Ligand

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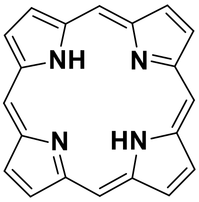
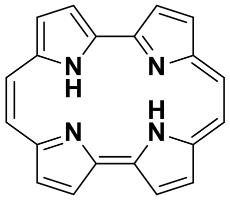
Abstract:

Porphycene, an 18π-aromatic rectangular tetrapyrrolic macrocycle, is the first constitutional isomer of porphyrin to be reported via McMurry type reductive self-coupling of bipyrrole dialdehydes by Vogel.[1] In spite of its superior ability as a therapeutic in photodynamic therapy compared to porphyrin, the synthetic difficulties associated with the preparation of bipyrroles limited the development of porphycene chemistry.[2] The presence of two bipyrrolic units make porphycene more responsive towards the effect of substitution than its parent isomer.[3] Our efforts towards exploiting this attribute towards tuning the photophysical, structural and coordination chemistry of porphycene unravel several unique features of this macrocycle will be elaborated.[4-5]



Porphyrin



Porphycene

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Professor Pradeepta K. Panda received his B.Sc. degree in Chemistry from Utkal University (Odisha) in 1990. He joined Indian Institute of Technology Kanpur (India) for his Master's degree. He pursued his doctoral research at the Indian Institute of Sciences, Bangalore (India) from 1994 to 2002. Then, he moved to South Korea as a Postdoctoral Fellow with Professor Chang-Hee Lee in the Kangwon National University for about three years (2002-2005). He then moved to Japan to join first as a Postdoctoral Fellow and subsequently as a JSPS Fellow with Professor Jun-ichiro Setsune at the Kobe University at Kobe (2005-2006) for about eighteen months. Soon he moved back to India to start his independent research career at the School of Chemistry, University of Hyderabad in 2007, where he is currently a full Professor. His research interests involve around fundamental and functional aspects of porphyrinoid chemistry. He has authored more than 60 independent research publications and three patents. He has successfully guided 13 Ph D students.

Prof. Kalyan K. Sadhu

Gold nanoparticle: classical to nonclassical growth

Kalyan K. Sadhu

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Abstract:

Primary or secondary nucleation during the gold nanoparticles growth depends upon the energy barrier and ligand concentration maintained during the reaction condition.[1] Seed-mediated synthesis methods are commonly known to prepare gold nanocrystals with controlled morphologies.[2] We have used amine modified DNAs for sequence dependent formation of gold nanoflowers and gold nanospheres using spherical gold nanoparticles as seeds.[3] Adsorption of amino acids or peptoids onto the surface of nanoparticles also offers a novel route to generation of nanoparticle assemblies with versatile gold nanoarchitectures.[4] Our recent observation related to methionine controlled nonclassical nucleation during growth reaction in presence of traditional citrate stabilized gold nanoparticle as seed.[5] The interaction between Au^+ with thioether functional group in methionine restrict the further reduction of Au^+ to Au^0. This nonclassical nucleation process has been further explored in the growth reaction with three methionine containing bio-inspired peptides.

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Kalyan K. Sadhu obtained his B.Sc. (Chemistry Hons.) and M.Sc. in Chemistry from **Presidency College, Kolkata,** affiliated with Calcutta University. He received his Ph.D. from the **IIT Kanpur in 2009**. After receiving his Ph.D., he joined **Osaka University**, Japan for two years as Specially Appointed Assistant Professor. Subsequently, he joined **University of Strasbourg for two years and then moved to University of Geneva** for one year as a postdoctoral fellow. He joined as an Assistant Professor in **Chemistry Department** at **Indian Institute of Technology Roorkee.** Currently he is working as an Associate Professor in the same department.

His group is working in Nanobio Interfacial Chemistry & Chemical Biology with a primary focus on gold nano- and supra-architectures for biological applications such as imaging, recognition, and drug delivery. They are much engaged to find the role of amine modified single strand DNA structures into the formation of gold nanoflower. The roles of specific amino acids and their interactions with gold nanoparticles are currently also focused for the detection of single mutation in the peptide sequence.

Prof. Chandan Mukherjee

Bare and Porous Silica Nanosphere-Confined Thermodynamically Stable Aquated Fe(III)- and Mn(II)-Complexex as Potential Dual-Mode MRI Contrast Agent

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Abstract:

Magnetic resonance imaging in the presence of contrast agents has emerged as an indispensable imaging modality for the early-stage diagnosis of many diseases. Nevertheless, the development of stable contrast agents with a high relaxivity remained as the primary challenge. In this endeavor, mononuclear, aquated, thermodynamically stable Fe(III) and Mn(II) complexes of hexadentate chelating ligands have been explored. The concentration-dependent changes in the image intensities in T_1- and T_2-weighted phantom images put forward the biocompatible complexes as a potential dual-mode MRI contrast agent. Furthermore, the organ specific *in vivo* studies have reinforced the applicability of the newly established systems. The synthesis and contrast ability of the developed new bare and porous silica nanosphere entrapped systems would be discussed in detail.

Curriculum Vitae		
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Current Position	Professor Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati-781039, Assam, India	
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Experience (Past Employment History)	August 2019- Present February 2015-August 2019 April 2011-February 2015 November 2010-March 2011 February 2007-August 2010 July 2006-January 2007 August 2003 –June 2006	**Professor** *Indian Institute of Technology Guwahati* **Associate Professor** *Indian Institute of Technology Guwahati* **Assistant Professor** *Indian Institute of Technology Guwahati* **Assistant Professor** *The Tokyo University, Tokyo, Japan* **Postdoctoral Research in Chemistry** *Universität Bielefeld, Germany, Germany* **Postdoctoral Research in Chemistry** *Max-Planck-Institut für Bioanorganische Chemie, Germany* **Doctoral Work** *Max-Planck-Institut für Bioanorganische Chemie, Germany*
Awards & Fellowships	➢ Associate, Indian Academy of Science, Bangalore (2015-2018). ➢ DFG-Fellowship for postdoctoral study (2007-2010, German Research Society). ➢ DFG -Fellowship for doctoral study (2003-2006, German Research Society). ➢ National Scholarship (2001, Govt. of India). ➢ National Scholarship (1998, Govt. of India).	

Prof. Soma Mukherjee

Small-Molecule Luminescent Chemosensors: Fascinating Chemistry and Sustainable Applications

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Abstract:

The present work focuses on the design and development of new and selective small-molecule luminescent chemosensors using hydrazone and Schiff base moieties. Considerable attention has been placed to explore new synthetic routes, sustainable reagents and non-destructive techniques for rapid sensing and monitoring of environmental pollutants. Most of them offer good solubility, low detection limit, high sensitivity, rapid response time and high quantum yield. The proposed sensing mechanism supported by 1H NMR and DFT calculations have been carried out. The performance of chemosensors with respect to sensitivity, linear range, limit of detection, selectivity, stability etc. are studied. Moreover, structural diversities, versatile photophysical properties, biocompatibility, easy synthesis of these chemosensors might facilitate various applications like on-site and real time detection, monitoring of multicomponent analytes without prior separation, reversibility, simultaneous selctive extraction and recovery of trace metals, non-destructive analysis, logic gates detection algorithm etc. to reduce the risk and environmental footprint. The basic principles involved in the design of chemosensors for specific analytes alongwith problems and challenges in the field as well as possible future research directions are also covered.

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Name: Prof. (Dr.) Soma Mukherjee

Designation: Professor

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Academic Background: M.Sc.; Ph.D.

The Ph.D. work was carried out at the Dept. of Inorganic Chemistry, Indian Association for the Cultivation of Science, Jadavpur, Kolkata under the supervision of Prof. Animesh Chakravorty, Distinguished Emeritus Professor, Dept. of Inorganic Chemistry, Indian Association for the Cultivation of Science (IACS), Jadavpur.

Thesis Title:

Studies on Transition Metal Chemistry of Some ONS Ligands. The post-doctoral research work was carried out at the IACS, Jadavpur on coordination chemistry.

Research Area:

Coordination Chemistry, Environmental Chemistry, Environmental Quality Monitoring and Management, Molecular Recognition, Spectroscopy, Pollution Studies.

Ongoing Research Statement:

- **Total Publications:** 86
- **Peer Reviewed Journal Publications**: 51 (International- 41, National-10)
- **Full Paper in Conference Proceedings**: 35
- **Total Citations**: 860 **Average Impact Factor**: 3.0
- ***h*-index**: 20 ***i10*-index**: 32

Prof. Sk. Jasimuddin

Electrocatalytic Water Oxidation by Heterogenized Manganese Complexes

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Abstract:

Development of efficient and robust water oxidation catalysts (WOCs) is a key challenge of the overall water splitting process. Nature employs an oxygen evolving complex (OEC) composed of a manganese cluster, $CaMn_4O_5$ in photosystem II to catalyse the oxidation of water. Since the discovery of the OEC (PS II), extensive research effort has been dedicated to the development of manganese-based artificial water oxidation catalysts, along with other transition metal based WOCs. Till date, a good number of homogeneous electrocatalysts based on manganese complexes have been reported to catalyse water oxidation reactions, but the main drawback is their poor stability and high overpotential. To enhance the robustness and catalytic activity, heterogenization of the molecular complex by covalent or non-covalent binding to a solid surface is a good choice. Recently, we have developed a few manganese complexes based heterogeneous electrocatalysts and obtained encouraging results. An overview of our work will be highlighted in this conference.

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Sk. Jasimuddin is Professor of Chemistry at Assam University, Silchar (A Central University) where he has been a member of the faculty since 2005. He received his Ph.D. in Chemistry for research supervised by Professor Chittranjan Sinha in the field of Coordination Chemistry at the University of Burdwan in Bardhaman and did postdoctoral research with Professor Joe Otsuki in the field of photocatalysis at the College of Science and Technology, Nihon University, Tokyo, Japan. He has published several research articles in reputed national and international journals. His current research interests include electrocatalytic/ photo-electrocatalytic water oxidation reaction and electrochemical sensing of bio-molecules and organic pollutants.

Dr. Subhadip Neogi

Exploring the pore-chemistry in crystalline frameworks through task-specific functionalization

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Abstract:

Metal–organic frameworks (MOFs) and covalent organic frameworks (COFs) are crystalline porous materials that caused a renaissance in recent times because of their structural diversity, remarkable surface area, thermo-chemical stability, and wide range of potential applications.[1] In particular, task-specific modulation of pore chemistry in these frameworks can lead to effective separation and mild-condition chemical conversion of carbon dioxide (CO_2).[2] Functionality engineering in these materials also benefit ultrasensitive detection and de-toxification of harmful organo-toxins[3] as well as atom-economic cross-coupling reactions.[4] This presentation will cover most-recent research works of framework chemistry group at CSIR-CSMCRI, which aim systematic functional-tagging in hybrid and organic porous frameworks for environmental remediation and sustainable catalysis.

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1. (a) H. Furukawa, K. E. Cordova, M. O'Keeffe, O. M. Yaghi, *Science*, **2013**, *341*, 1230444. (b) X. Guan, F. Chen, Q. Fang, S. Qiu, *Chem. Soc. Rev.*, **2020**, *49*, 1357-1384.
2. (a) N. Seal, S. Neogi, *ACS Appl. Mater. Interfaces*, **2021**, *13*, 55123–55135, (b) N. Seal, K. Karthick, M. Singh, S. Kundu, S. Neogi, *Chem. Eng. J.*, **2022**, *429*, 132301.
3. (a) R. Goswami, S. Das, N. Seal, B. Pathak, S. Neogi, *ACS Appl. Mater. Interfaces*, **2021**, 13, 34012-34026. (b) R. Goswami, B. D. Bankar, S. Rajput, N. Seal, R. Pillai, A. V. Biradar, S. Neogi *J. Mater. Chem. A*, **2022**, *10*, 4316-4332.
4. (a) G. Kumar, M. Singh, R. Goswami, S. Neogi, *ACS Appl. Mater. Interfaces*, **2020**, *12*, 48642–48653. (b) G. Kumar, R. S. Pillai, N. H. Khan, S. Neogi, *Appl. Catal. B-Environ.*, **2021**, *292*, 120149.

Dr. Subhadip Neogi received his Ph.D. from I.I.T. Kanpur under the supervision of Prof. P. K. Bharadwaj. After NRF Post-doctoral Fellowship with Prof. L. J. Barbour (Stellenbosch University, South Africa) he joined Prof. M. Schmittel (University of Siegen, Germany) as Humboldt Post-doctoral Fellow. Dr. Neogi received **DST Young Scientist Award** in 2012 and **Early Career Research Award** in 2016. He is life-fellow of Alexander *von* Humboldt Foundation, Indian Chemical Society. He has supervised four Ph.D. students, and three students are presently working in his research group at CSIR-CSMCRI. Dr. Neogi authored 62 International Research papers and has been recognised as top 3% cited ACS Author in 2021 for all publications from India.

Major research areas:

Metal-Organic Frameworks and Covalent Organic Frameworks, Gas adsorption, Toxic Pollutant Monitoring and Anticounterfeiting Applications, Heterogeneous Catalysis

Selected recent publications:

1. N. Seal, **S. Neogi** *ACS Appl. Mater. Interfaces*, **2021**, *13*, 55123–55135.
2. G. Kumar, R. S. Pillai, N. H. Khan, **S. Neogi** *Appl. Catal. B-Environ.*, **2021**, *292,* 120149.
3. R. Goswami, S. Das, N. Seal, B. Pathak, **S. Neogi** *ACS Appl. Mater. Interfaces*, **2021**, *13*, 34012-34026.
4. N. Seal, A. S. Palakkal, M. Singh, R. Goswami, R. S. Pillai, S. Neogi *ACS Appl. Mater. Interfaces*, **2021**, *13*, 28378-28389.
5. M. Singh, A. S. Palakkal, R. S. Pillai, S. Neogi *J. Mater. Chem. C*, **2021**, *9*, 7142-7153.
6. R. Goswami, K. Karthick, S. Das, S. Rajput, N. Seal, B. Pathak, S. Kundu, **S. Neogi** *ACS Appl. Mater. Interfaces*, **2022**, *14*, 29773-29787**.**
7. *M. Singh, S. Neogi Inorg. Chem.* ***2022****, 61, 10731–10742.*
8. **R. Goswami**, B. D. Bankar, S. Rajput, N. Seal, R. Pillai, A. V. Biradar, **S. Neogi** *J. Mater. Chem. A*, **2022**, *10*, 4316-4332.
9. M. Singh, S. Neogi, *Inorg. Chem. Front.*, **2022**, 9, 1897-1911

N. Seal, K. Karthick, M. Singh, S. Kundu, **S. Neogi** *Chem. Eng. J.*, **2022**, *429*, 132301

Prof. Subhendu Naskar

Single site Ruthenium Complexes with anionic ligands as Molecular Water Oxidation Catalysts

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Abstract:

Investigation on single site Ruthenium complexes gained acceleration in last decade after the experience of synthetic complexity of binuclear blue dimer analogues.[1-3] In the mono nuclear family, molecules with anionic ligands (pyridine 2 carboxylate and pyrazine 2 carboxylate) have been found to be more effective than the neutral one. Herein we report different heteroleptic mononuclear Ru^{II} and Ru^{III} complexes with anionic ligands. The complexes have been screened for the chemical (by CAN) and electrochemical water oxidation. LSV, CV, and bulk electrolysis study measures the electrocatalytic activity. A systematic variation in terms of electron donating and withdrawing property on the ligand scaffold has been found to display a profound effect on the rate of electrocatalytic oxygen evolution. The underlying mechanism has been elucidated by means of chemical, electrochemical and theoretical (DFT) data. At pH = 1, maximum turnover frequency (TOF_{max}) has been experimentally obtained from the foot of wave analysis (FOWA).

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Academic & Research: Dr. Naskar obtained his B.Sc & MSc in chemistry from University of Calcutta and PhD degree from IIEST-Shibpur in 2006. Then he moved to ICMMO, University of Paris-11, Orsay for a post doctoral position. In 2008 he started independent research as young scientist in the DST Fast Track Scheme in June'2008. In Aug'2009 Dr. Naskar joined Department of Chemistry, Birla Institute of Technology-Mesra, Ranchi as Assistant Professor. In 2020 he was promoted to Associate Professor in the same place.

His major research area is Coordination Chemistry and its applications to biologically relevant systems. For last few years the group is focusing on the artificial Photosynthesis based Energy production: development of molecular water oxidation catalysts as well as proton and carbon dioxide reduction catalysts. Till now Dr. Naskar and his group has published 45 research articles in reputed journals. He has successfully completed 5 projects from different government grant Agency, e.g., DST, UGC, CSIR, AICTE and SERB.

Prof. Sujit K. Ghosh

Uranium Extraction from (Sea)Water: Its Significance in the field of Clean Energy and Safe Drinking Water

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Abstract:

With rising global energy demand and environmental concerns associated with fossil fuels, sustainable energy supply to the global community remains a great challenge. Amongst the mature and efficient clean energy technologies, presumably, nuclear power will remain the sole existing reliable energy source in the future, as anticipated by the International Atomic Energy Agency (IAEA). Recently, uranium extraction from seawater (UES) is considered one of the seven chemical separations, which have the potential to change the world.1 However, uranium recovery from seawater is extremely challenging due to its ultra-low concentration (~3.3 ppb). On the other hand, Uranium (U) contamination of groundwater is another major concern due to its toxic nature. Given the paramount importance, uranium extraction from seawater and groundwater from energy and environmental point of view has great significance and is an important current research topic. I will discuss about highly selective and efficient Uranium extraction from natural seawater and ground water by a functional metal-organic framework (MOF) for potential applications of Uranium as renewable, clean and green energy source and for safe drinking water. [2-3].

Figure: Advanced porous materials as efficient scavenger of targeted metal ions from water.

References:

1) D. S. Sholl and R. P. Lively, **Nature, 2016**, 532, 435. 2) **Book**: *Metal-Organic Frameworks (MOFs) for Environmental Applications* 1st Ed. (**Ed.: S K. Ghosh**), Elsevier, **2019**, https://doi.org/10.1016/C2017-0-01721-4. 3) Mollick, S.; Saurabh, S.; More, Y.D.; Fajal, S.; Shirolkar, M. M.; Mandal, W.; Sujit K. Ghosh, S. K.; ***Energy & Environmental Science*** **2022**,15, 3462-3469.

Prof. Sujit K. Ghosh

Department of Chemistry, IISER Pune, India

Education:

PhD (Chemistry), IIT Kanpur in 2006

Positions Held:

☐ 2020- Professor, IISER Pune

☐ 2009-2020 Assistant and Associate Professor, IISER Pune

Research Interests:

☐ Advanced functional porous materials

☐ Materials for clean energy and safe drinking water.

☐ Industrially relevant chemicals separation.

Publications and Citations Summary:

Sum of the Times Cited: **> 12550; h-index: 57**

Total Number of Publications: **> 150**

Average impact factor per article: > 8.5

Average citation per article: > 80

Selected Awards and Honours:

☐ Chemical Research Society of India (CRSI) Bronze Medal.

☐ International advisory board of the journals ChemComm. And ChemPlusChem

☐ Materials Research Society of India (MRSI) Medal.

☐ India Research Excellence - Citation Award by Clarivate Analytics.

☐ Alexander von Humboldt (AvH) Fellowship for Experienced Researchers, Germany.

☐ Young scientist awards by INSA, NASI, IASc, DAE, Alkyl Amines-ICT, AVRA.

☐ Newton International Fellowship, UK. (Offer declined).

☐ JSPS Post-Doctoral Research Fellowship, Japan.

Prof. Sabyasachi Sarkar

Nitrogen fixation, our effort in the past 5 decades finally succeeded to mimic Nature

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Abstract:

Since mid-seventies we tried to understand how Nature under ambient conditions transform one nitrogen molecule to two ammonia. We (also others) tried ab initio to create molecular assembly using Mo, Fe, and S which will possess the essence of the Mo-Fe cofactor responsible for catalytic activity. But demonstration of catalytic activity similar to the native protein failed. Several questions were raised like how thermodynamics allow at a time to pump minimum 6 electrons (in reality 8 electrons) to this site. Like an electric circuit, which may have charging condenser, here iron-sulfur cluster containing proteins store electrons from simple electron generating molecules (ATP/NAD(P)H) those can be properly switched to the active site once the nitrogen molecule is attached to flush all the electrons at a time satisfying the ease of its multi-electron reduction following, $-\Delta G = nFE$. Nature invoked such principle but the structure of active cluster (co-factor) is very fragile. It is supported by a large network of apo protein to induce overall stability of the holoprotein during catalytic turnover reaction. Several electrostatic/hydrogen bonding act as switches in helping its catalytic role by regulating the directional electron flow using off and on mode. We finally used homemade flexible nanocarbon network to mimic the role of apo protein. This supports the fragile all iron (similar to Mo-Fe or V-Fe cofactor) active site created in-situ. We demonstrate that with such an assembly the production of ammonia under ambient condition in aqueous medium is achieved.

Dr. Sabyasachi Sarkar, Distinguished Honorary Professor, Ramakrishna Mission Vidyamandira, BelurMath; Honorary Visiting Professor, Indian Institute of Science and Technology-Shibpur, Botanic Garden, Howrah, West Bengal and Formerly Senior Professor and Head, Chemistry Department of IIT Kanpur continuing research over 50 years in the diversified fields like : Chemical Darwinism, extant life from Archaeal hyperthermophiles to latest mesophiles. Trapping solar energy by designing synthetic leaf; oxidative stress related reactive oxygen and nitrogen species, modelling hydrogenases for energy and non-invasive bioimaging by non-toxic water-soluble fluorescent nano-carbon onions and graphene oxide used in in vivo drug carrier and delivery including crossing blood brain barrier. Shown Atherosclerosis by TMAO of gut microbiota. Designed nano carbons applied to young plants in conserving water and fertilizer for their optimized use enhancing fruits and bio mass. Demonstrated to control mosquito breeding using nano carbon non evasivelynto prevent mosquito vectors of infectious diseases. He has shown architectural marvel in silk cocoon with the natural thermostatic and humidity control with preferential oxygen gating inside cocoon suggesting the construction of greenhouse architecture. Also demonstrated soft magnetic memory of silk cocoon membrane and the role of nano iron sulfide as plant growth booster and super capacitor. He has developed low-cost nano carbon technology to desalinate water with remedial of arsenic and fluoride from water and also shown the anthropogenic nano carbon in aerosols creating global climate change, warming, winter smog and breathing problem. He mapped the degradation of Taj Mahal. Presently doing research on trapping radiant energy of the earth beyond visible light and the use of low-cost nano carbon to combat RNA viruses including corona.

Professor Sarkar guided 46 PhD and more than 200 Master theses with over 250 research publications in refereed journals, and made five US, one European Union, one Chinese and three Indian patents. He writes popular scientific articles in English and in Bengali and short stories with satire in Bengali.

Homepage:http://home.iitk.ac.in/~abya/ ,
https://en.wikipedia.org/wiki/Sabyasachi_Sarkar

Dr. Biswajit Dey

Multi-Functional Supramolecular Gel for Nano, Nano-bio and Biological Applications

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Abstract:

The supramolecular chemistry is developing quickly due to its astonishing role in biological world. Nature greatly adores the supramolecular occurrences. Scientist is focusing to develop the man-made supramolecular architectures rather than serendipity by following the aspect of natural bio-specifications. Various intriguing non-covalent type interactions like hydrogen-bonding, electrostatic, hydrophobic, hydrophilic, van der Waals forces, aryl-system based interactions, metal-ligand interactions are playing the main factor for the formation of stable supramolecular architectures. Crystals, 2D materials, inorganic-organic hybrids, metal-organic materials, soft-gels are encompassed in the domain of supramolecular networks. The mechanical flexibility and viscoelasticity of the gel specifically the water-based hydrogel receives a critical attention to generate versatile multi-functional materials. In this present approach, several 2D nano materials involving Molybdenum dichalcogenides like MoS_2, $MoSe_2$, WS_2, hexagonal (BN), Graphene Oxide based metallogel, metallohydrogel and hydrogel scaffolds are synthesised and the physical, chemical and biological applications of these gel-nano composites are explored. Gel-nano composites based semiconducting opto-electronic devices are also developed. GO, MoS_2 and $MoSe_2$ dispersed tertrapyridine moiety based supramolecular hydrogel-scaffolds are synthesised and used for the stabilization of 'Green' bio-functional Ag-NPs. The efficient strategy of evolving the GO dispersed supramolecular hydrogel directed DNA-GO-hydrogel stuff has also been explored for the nano-bio composites formation. The formation and stabilization of GO-DNA-hydrogel based 'Green' Ag-NPs are also explored.

Dr. Biswajit Dey is serving as the Assistant Professor, Department of Chemistry, Visva-Bharati (A Central University), Santiniketan, West Bengal, India. He did his B.Sc.(H), M.Sc. and Ph.D. from Jadavpur University. He has published 51 papers in the international journals of American Chemical society, Royal Society of Chemistry, Elsevier, Wiley, Springer. The average impact factor of his publication is more than 4. He presented more than 35 International and national level conferences. He acted as the external Board of Study member of Amity University, Ranchi. He served as the esteemed reviewers of more than 100 journals of several international and national journals societies including American Chemical society, Royal Society of Chemistry, Elsevier, Wiley, Springer, MDPI, etc. Presently he is serving as the Associated Editor for Chemistry Africa (Springer Journal), an international journal. He produced 5 Ph.D. scholars. He has research experience of more than 17 years. He has one Indian Patent on indigenous technology for industrial purposes granted on 11th October, 2022. He has completed three research projects of SERB-DST, CSIR and West Bengal DST & Biotechnology. He acts as the reviewer of international research projects. His special research interest is to explore the supramolecular systems including crystals, co-crystal, metallogels, organogels, metallohydrogels, bio-macromolecule based gels, self-healing stuff, 2D nano materials, transition metal dichalcogenides, Non-linear optical materials, sensor, semiconducting diodes, catalysis, nano-bio technology.

Prof. Debasis Dhak

Water Purification, Waste Water Treatment Using Nanomaterials: Metal Oxides and Metal-Organic-Frameworks

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Abstract:

Rising population and urbanization have escalated the global demand for adequate, safe and easily available water resources. Rapid industrialization and climate change and huge human population emerge a serious crisis of water availability and waste water management. To overcome the crisis of sustainable water resources and waste water management, focusing on challenges are utmost necessary. Sustainable waste water management has become the primary agenda on the Sustainable Development Goals worldwide. Therefore, purification of drinking water through the removal of heavy metals, non-metals, and other organic toxicants etc as well as waste water treatment through adoption of green and sustainable chemical process and subsequent managements are the major challenges. The presentation will focus on an opportunity to review and address innovations, research on water purification using nanomaterials: metal oxides and metal-organic-frameworks.

Dr. DEBASIS DHAK
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MSc.:Visva-Bharati University, 2002
B.Sc.: Visva-Bharati University, 2000
Post Doc: University of British Columbia, Canada (2008-2010)
Teaching Experience:
Assistant Professor (2006-2012): Department of Chemistry, Serampore College, Hooghly
Assistant Professor (20013-2018): Department of Chemistry, Sidho-Kanho-Birsha UniversityPurulia
Associate Professor (2018-2019): Associate Professor, SKBU
Professor: March 2019-till date
Awards:
Received **Siksha-Ratna** award from Govt. of West Bengal in 2020
Received **Young Scientist** Fast Track Project from DST, New Delhi in 2012
Received two **travel grant** award for attending international conferences
Received **National Fellowship** award during study from Xth plus to PG level.
8 Best Poster and Oral presentation award to the research students
2 Anveshan award to the research students organized by Association of Indian Universities
Associate Guest Editors: **Journal of Nanomaterials**, (Hindwai Publisher, Impact Factor: 2.98)
Frontiers in Chemistry (Impact Factor: 5.22)
Guest Editor: **Journal of the Indian Chemical Society**(Formerly Indian Chemical Society, now Elsevier)
Life Member:
Materials Research Society of India,
International Association of Advanced Materials,
Indian Chemical Society
Alumni member of Indian Institute of Technology Kharagpur
Books: 2 (international), Book Chapters: 6
Papers: 76 (International) Ph.D awarded: 1 No. of Current Ph.D. Students: 8 Reviewer of many journals of Elsevier, ACS, Springer, RSC,Taylor and Francis, etc.
Current Project as PI: 11 lakhs, As Co-PI: 5.68 Crore
Research areas:
Water treatment (Fluoride removal),
Waste water treatment &management (Industrial dye waste),
Ferroelectric energy storage materials etc.
Technology Developed:
Prepared **Fluoride free water filter candle** using Nano-adsorbent developed and synthesized in laboratory at SKBU.
Patents: 1 Patent granted (South Africa) and 2 Indian Patent Processing

Stabilization of M(III) (M = Co, Ni, Cu) with Newly Designed Pentadenate Azo-Amide Ligand

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[b]Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur India
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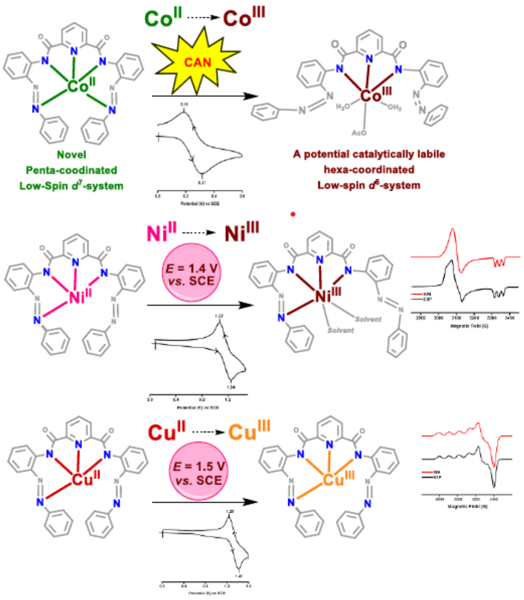
Abstract:

A new pentadentate azo containing amide ligand of biological importance1,2 has been prepared. Four low-spin metal (metal = Co, Ni, Cu) complexes were synthesized, structurally, and spectroscopically characterized, along with DFT and TD-DFT calculations. The non-innocent ligand binds with Co(II) in a rare penta-coordinated fashion in its low-spin state, utilizing all potential donor sites. Chemically and electronically oxidized Co(III), Ni(III) and Cu(III) species were successfully achieved and characterized. Co(III) can act as a potential catalyst3 due to its weakly coordinated solvents and acetate ions in three of the six coordination sites. Ease of stabilization2 of M(II) and M(III) with variable coordination geometry presents its unique prospect in catalysis and biomimicking action of bleomycin-type anti-cancer drugs.



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Structural, thermal, and optical analysis of a Mg(H2O)6 based supramolecular hydrogen bonded framework

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Abstract:

In this endeavor the crystal structure, the thermal and optical properties of {[Cu(II)(2,3-pdc)].[Mg(H2O)6].(H2O)}n, (where, 2,3-pdc = 2,3-pyridine dicarboxylate), synthesized by reflux method have been reported. The complex is a supramolecular hydrogen bonded framework [1] with triclinic $P1$ space group. The π-π interaction[2]between the different pdc rings of adjacent 1D chains of the complex forms the 2D anionic sheet which are further connected by guest water mediated hydrogen bonding interactions with the cationic units to form the 3D supramolecular architecture [Fig.1]. The phase purity of the complex is checked by PXRD. According to thermo gravimetric analysis, the complex contains both guest and coordinated water molecules.The transition due to copper in octahedral coordination geometry is observed in UV-Vis spectra [3]. Presence of both coordinated and uncoordinated carboxylic acid groups and hydrogen bonded water molecules is found in IR spectra [4]. Further studies on electrical properties of the complex are in progress.

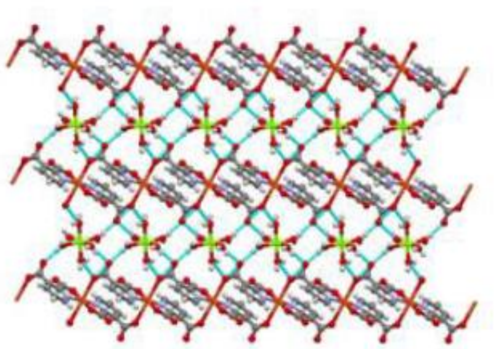

Fig.1: The 3D supramolecular architecture of the complex.

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Crystal structure of heterovalent Cu5AsO5F5

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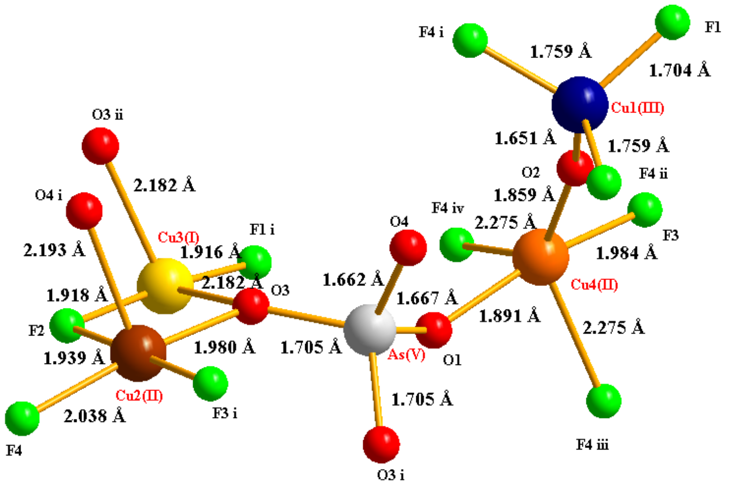
Abstract:

Cu5AsO5F5 [Cu3(II)Cu(III)Cu(I)As(V)O5F5] is new lineage of oxyfluoride[1] family where Copper exists in three different oxidation state as Cu(I), Cu(II) and Cu (III) and arsenic exist as arsenate(V)[2]. The resultant oxyfluoride has been synthesized via simple hydrothermal method. The basic geometry of the Cu5AsO5F5 was studied by single crystal X-Ray diffraction study. The asymmetric unit consist of three tetracoordinated units of [Cu1(III)OF3], [Cu3(I)O2F2] and [As(V)O4], and two pentacoordinated units of [Cu2(II)O2F3] and [Cu4(II)O2F3]. [Cu3(I)-O3-Cu2(II)-F2-Cu3(I)] forms a four membered ring, while [Cu1(III)-O2-Cu4(II)] forms a long chain in the basic unit. Both the four membered ring and long chain is connected through the [As(V)O4] unit. The contour diagram shows the different electron densities around the different Cu atoms. The resultant compound was further characterized by FTIR and SEM. Theoretical calculation was done by DFT. The DFT analysis provides an explanation for the structure as well as the atomic coordinates, hybridizations, and FTIR measurements, all of which are comparable to experimental data.



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Keywords: Hydrothermal synthesis**,** Oxyfluoride**,** Single crystal X-ray diffraction

Mononuclear Fe(III) complexes with phenol-based ligand: Synthesis, Structure, Catechol oxidase activity and as Amino acid sensing agent

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Abstract:

Fe(III) complex (**1**) of a sterically constrained phenol-based tetradentate N2O2 ligand *N,N′*-dimethyl-*N,N′*-bi(2-hydroxy-3,5-dichlorobenzyl)-ethylenediamine (**H2L**) have been reported. Benzoylacetone has been used as ancillary ligands to obtain the mixed ligand mononuclear complexes **[FeIIIL(bzac)]** (**1**). The syntheses, X-ray structures, spectroscopic studies and catechol oxidase activity of these complexes are described. Fe(III) complex crystallizes in monoclinic space group P21/n with a = 9.2164 Å, b = 16.5872 Å and c = 18.3092 Å. Fe(III) complex performs as an amino acid sensor material as well as an effective catalyst towards the oxidation of 3,5-di-tert-butylcatechol in methanol solvent. Both the absorption spectral analysis reveals that the complex has peaks at 484 nm due to ligand to metal charge transfer (LMCT) and emission spectra have a peak at 566 nm. In presence of Histidine, there is a red-shift about 70 nm and peaks arises about 564 nm while the emission spectra shows that the peak at 566 nm disappears completely and a new peak at 603 nm appears.

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A multifunctional catenated host for efficient binding of Eu3+ and Gd3+

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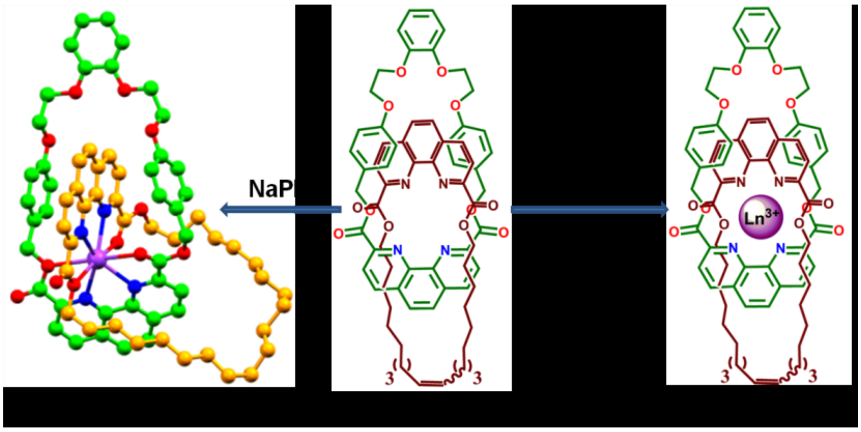
Abstract:

In recent decades, strategically designed mechanically interlocked molecules (MIMs) such as rotaxanes and catenanes have been emerged as potentially active prototypes in the modern scientific field.1-2 Such MIMs having three-dimensional coordination spheres, can be tuned in a unique topological manner to act as a flexible receptor to clasp selective ions/molecules in the chemically active pocket.3 In this context, we have reported the first example of a multifunctional **[2]catenane**, composed of phenanthroline (phen), ester and oxy ether functionalities, utilised for the binding of trivalent lanthanide metal ions such as Eu3+ and Gd3+.4 Towards the synthesis of catenated host systems, phen-ester- group embedded a new heteroditopic macrocycle (**PhenMC)** and an alkene terminated ligand (**Axle**) have been designed in such a way to compliment the binding preference of lanthanide metal ions with high coordination numbers. Finally, the interlocked structure of the catenane is confirmed *via* X-ray crystallography analysis of Na+ complex of **CATN**.



Keywords: Catenane, Lanthanides, Host-Guest, Phenanthroline, Multifunctional

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Synthesis and characterization of mononuclear dioxomolybdenum(VI) complexes with ONO donor ligand: Crystal structure, Protein binding studies and anticancer activities

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Abstract:

A series of new mononuclear dioxomolybdenum(VI) complexes having general formula MoO2L(D) [where D= CH3OH(**1**), Py(**2**), γ-pic(**3**), imz(**4**), 1-methimz(**5**)] have been synthesized by the reaction of MoO2(acac)2 with ONO donor shiff base ligand (H2L) obtained by the condensation of 2,4-dihydroxoacetophenone with anthranyl hydrazide. The complexes have been characterized by elemental analyses, various spectroscopic techniques. Crystal structures of the two complexes MoO2L(CH3OH) (**1**) and MoO2L(1-methimz)(**5**) were determined by the single crystal X-ray diffraction which reveal that each molybdenum centre in the complexes adopts a distorted octahedral geometry. The complexes give rise to interesting supramolecular architectures via hydrogen bonding and C-H···π interactions. The binding properties of the ligand and the complexes with BSA protein were investigated by absorption and fluorescence titration. The anticancer activities of the complexes were examined against human breast adenocarcinoma MCF-7 cell line. The complexes showed higher anticancer activities towards the cancer cell than the free ligand.

Halide-Specific Solid-State Stabilization of H5O2+ and Efficient Tuning of the Device-Performances of Semiconducting Photo-responsive Diodes

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Abstract:

Two different halides involving chloride and bromide assisted dissimilar crystalline supramolecular building blocks of 4′-(1*H*-imidazol-2-yl)-4,2′:6′,4′′-terpyridine (**ITP**) has been achieved. The π-systems of protonated pyridine and imidazole rings play a pivotal role for establishing the non-covalent π···π type supramolecular interactions in both the crystals and the π-system directed associations certainly assist to form the 3D supramolecular architectures of **ITP-Cl** and **ITP-Br** in solid-state. Most intriguingly, the supramolecular association of **ITP-Cl** uniquely stabilizes the cationic unit of hydroxonium hydrate (i.e. H5O2+) in the solid-state and such solid-state stabilization of H5O2+ by the imidazole-connected terpyridine based system is one of the pioneering challenges in crystal engineering. Distinctly, the hydrogen-bonded cluster-like assembly of H5O2+ and Cl- has been observed in **ITP-Cl** system through hydrogen donor-acceptor balance. Subsequently, a special drive has been endeavored to unveil the semiconducting feature including charge transport property and photo-responsive behavior of these synthesized **ITP-Cl** and **ITP-Br** based fabricated devices. Fascinatingly, the chloride mediated **ITP-Cl** based device shows remarkably higher electrical conductivity with respect to **ITP-Br** based device under photo-irradiation condition and this implies the tuning-effect of different halides towards the applicability of thin-film based device-performance. The device efficiency based experimental outcomes have been rationalized through the DFT-level analysis.

$Zn_3Sb_4O_6F_6$: Photocatalytic Activity, Knoevenagel condensation, and Bacterial Disinfection

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[a] Department of Chemistry, University of Kalyani, Nadia, West Bengal, India
[b] Department of Microbiology,University of Kalyani, Nadia, West Bengal, India

Abstract:

$Zn_3Sb_4O_6F_6$ crystallites have been prepared using a pH-regulated hydrothermal synthetic approach. This is the first [M-L-O-F] compound which has been employed in photocatalytic degradation of methylene blue dye and more than 80% dye degradation has been achieved within 3 hours using $Zn_3Sb_4O_6F_6$catalyst, synthesized at pH=3. Addition of 0.1 ml of 6% hydrogen peroxide accelerates the rate of dye degradation by around four times, resulting in more than 80% degradation within 60 mins using the catalyst, synthesized at pH=7. The direct band gaps (Eg) have been compared with different batch of $Zn_3Sb_4O_6F_6$, synthesized at pH=2 to 7, the lowest Eg was found to be 3.0 eV at pH=6, 7 while the band gap rises with lowering the pH and Eg = 3.6 eV was obtained at pH=2. The FESEM analysis depicts the change of surface morphology at different pH. $Zn_3Sb_4O_6F_6$ catalyzed Knoevenagel condensation processes yielded 99% product at 60oC in a solvent-free environment. The reaction has also been monitored with the reactant containing electron withdrawing and electron donating groups. The antimicrobial activities of the as prepared compound has been studied by 'Disk diffusion method' against a several known representative bacteria i.e., Enterobacter sp., Escherichia coli, Staphylococcus sp., Salmonella sp., Bacillus sp., Proteous sp., Pseudomonas sp., and Klebsiella sp. The crystal structure of $Zn_3Sb_4O_6F_6$ (Figure 1) has also been revisited which proved to be the identical crystal structure with cubic symmetry ($I\bar{4}3m$) as reported by Ali et al.1 All the above-mentioned activities were also tested on 6% KI doped $Zn_3Sb_4O_6F_6$ compound. The effect of dopant on $Zn_3Sb_4O_6F_6$ towards the variation of the aforementioned studies have also carried out.

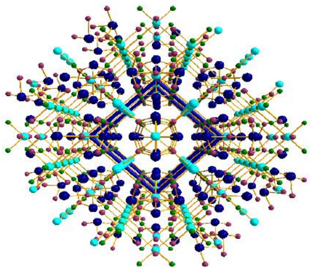

Figure 1: Crystal structure overview of $Zn_3Sb_4O_6F_6$

Reference:

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Keywords:

Hydrothermal Synthesis, Transition metal-oxyfluoride, Photocatalyst, Knoevenagel condensation, Bacterial disinfection

Synthesis, covalency parameters, energy calculations and Crystal features of Acylpyrazolone derived Pentavalent Uranyl complexes with DFT and Hirshfeld analysis

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Abstract:

Uranyl-acylpyrazolone complexes [UO2(PCBPMP)2(CH3CH2OH)] (**I**), [UO2(PCBMCPMP)2(CH3CH2OH)] (**II**), [UO2(PCBPTMP)2(CH3CH2OH)] (**III**), and [UO2(DMBPMP)2(EtOH)] (**IV**) were synthesized to analyze their pentagonal-bipyramidal geometry and covalency sequence **II**>**III**>**I**>**IV** mainly through the single-crystal XRD, 1H-NMR, TG-DTA, significant FTIR vibrations, and UV-Vis data. The covalency sequence mainly depends on stretching frequencies, average bond lengths of axial uranyl bonds and pentagonal equatorial plane, solvent coordination on a pentagonal plane, and kind of aryl group on nitrogen of pyrazolone ring. Sinha's covalency parameters were calculated from UV-Vis data, which shows that the covalency decreases in DMSO>DMF>Ethyl acetate>Ethanol>CHCl3 order. DFT calculations further gives evidence for covalency order through theoretical infrared frequencies and HOMO-LUMO gap. Theoretical bond properties were examined by calculating global index parameters. The Hirshfeld surface analysis was carried out to identify the crystal strength through interaction energies and energy frameworks in the ligand and intermolecular non-covalent surface interactions with fingerprint plots in both ligands and complexes.

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Design and synthesis of novel Zn(II) complexes as potential drug candidates against SARS CoV-2

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Abstract:

The aim of this study was to synthesis and molecular design of a series ofnovel Zn(II) complex complexes viz.[Zn(L)(en)]ClO4(**1**), [Zn(L)(bipy)]ClO4(**2**),[Zn(L)(phen)]ClO4 (**3**), [Zn(L)2] (**4**) as potential antivirus drug candidate against the S proteins of the SARS-CoV-2 and its Omicron variants [Scheme 1, where, HL = (Z)-N-phenyl-N'-((Z)-phenyl(pyridin-2-yl)methylene)carbamohydrazonic acid; en= ethylenediamine; bipy= 2,2’-bipyridyl, phen= 1, 10-phenanthroline]. They fully characterized, including single crystal X-ray crystallography. DFT calculations have been explored for structure-property relationship. The Hirshfeld surface analysiswas also performed.We have performed the molecular docking of Zn(II) complexes with SARS-CoV-2 Mpro(PDB ID: 7LM9)[1]and its Omicron variants(PDB ID: 7WOP)[2]. Molecular docking revealed the higher binding energy (ΔG)with good inhibition constant (Ki)for all the synthesized complexes. Overall, our in-silico molecular docking studies explored the potential role of Zn(II) complexeswhich may be used as antivirus drug candidates against SARS CoV-2 and its Omicron variants[3-5].

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N-(aryl)pyrrole-2-aldimine complexes of ruthenium: Synthesis, structure and, spectral and electrochemical properties

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Abstract:

Reaction of [Ru(dmso)$_4$Cl$_2$] with N-(4′-R-phenyl)pyrrole-2-aldimines (abbreviated as HL-R; where H depicts the dissociable pyrrole N-H proton and R = OCH$_3$, CH$_3$, H and Cl) in refluxing toluene in the presence of triethylamine has afforded a family of complexes of type [Ru(L-R)$_2$(dmso)$_2$]. Crystal structures of all the four complexes have been determined, which show that the aldimine ligands are chelated to the metal center as N,N-donor and the dmso's are coordinated through sulfur. Relative thermodynamic stability of the five possible geometric isomers of these complexes has been assessed with the help of DFT calculations, and the *tcc*-isomer (*tcc* depicting the pyrrole-nitrogens to be *trans*, the imine-nitrogens *cis*, and the S-coordinated dmso's *cis*) is found to be the most stable isomer. The isolated complexes also have the *tcc* geometry, as observed in their crystal structures. The coordinated dmso's are found to be displaceable by chelating bidentate ligands (depicted as L-L) to furnish mixed-tris complexes of type [Ru(L-R)2(L-L)], as demonstrated through isolation of two such complexes (with R = OCH3, and L-L = 2,2′-bipyridine or 1,10-phenanthroline). Optimization of their structures and probing into the thermodynamics of their formation have been done by DFT method. Electronic spectra of all six complexes, recorded in dichloromethane solution, show intense absorptions in the visible and ultraviolet regions, which have been analyzed by TDDFT method. Cyclic votammetry of all the complexes in acetonitrile solution shows ruthenium based oxidative response(s) within 0.77-1.24 V vs SCE, and ligand (bpy/phen) based reductions within -1.06 to -1.70 V vs SCE in case of the [Ru(L-R)$_2$(L-L)] complexes.

Bis(catecholato)germane: an effective catalyst for Friedel–Crafts alkylation reaction

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Abstract:

An air-stable and storable Bis(catecholato)germane; $[Ge^{IV}(C_6H_4O_2)_2(H_2O)_2]$ **(1)**, was synthesized by the reaction of catechol and germanium oxide in water. Complex 1 was characterized by FT-IR spectroscopy, NMR spectroscopy, mass spectrometry, and elemental analysis. Complex 1 was employed as a Lewis acid catalyst in the Friedel–Crafts alkylation reaction of indole with various aldehydes and β-nitrostyrene derivatives separately. The yield of the product for the formation of bis(indolyl)alkanes and nitro-alkylated indoles was up to 95% and 96%, respectively. All isolated catalytic organic products were characterized by ^{1} H and ^{13}C{^{1} H} NMR spectroscopy and mass spectrometry. These observations confirmed the catalytic efficacy of complex 1 as a Lewis acid in both reactions. Based on the experimental findings, a plausible mechanism is proposed for both reactions.

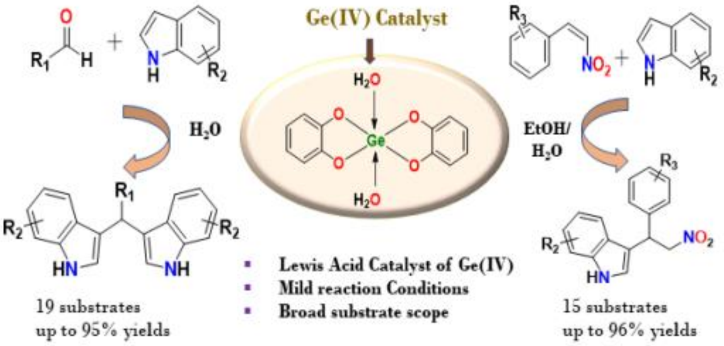

Figure: Bis(catecholato)germane as a Lewis-acid catalyst for Friedel-Crafts alkylation reaction.

Keywords: Germanium(IV) complex; Homogeneous catalysis; Main Group catalyst; Lewis acid.

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Synthesis double oximato dinuclearcopper(II)its its phenoxazinone synthase mimicking activity

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Abstract:

A dinuclear copper(II) complex, $[(CH_3CN)Cu(L)_2Cu](ClO_4)_2$, has been synthesized by reacting an oxime based tridentate Schiff base ligand, 3-[2- (dimethylamino)-ethylimino] butan-2-one oxime (HL), with copper(II) perchlorate hexahydrate. The complex has been characterized by elemental and spectral analyses. Structure of the complex has been confirmed by single crystal X-ray diffraction technique. The complex may be used as moderate catalyst for the oxidation of o-aminophenol to 2-aminophenoxazine-3-one.

Exploration of Variable Temperature Magnetism and Electrical Property of a 3D Mn(II)- MOF

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Abstract:

In this current trend of technology dependent civilization multifunctional applicability of coordination polymers (CPs) are highly stimulating. In search of such chemical compounds, a Mn(II) coordinated MOF has been designed. The structure determination of $\{[Mn_2(tdc)_2(pcih)_2(EtOH)]_n\}$ **(1)(H$_2$tdc**=2,5-thiophene dicarboxylic acid, **pcih**=Pyridine-4-carboxaldehyde isonicotinoyl hydrazone) has revealed the formation of 3D supramolecular architecture via the combined nearly perpendicular bridging of **pcih** and **tdc^{2-}** ligands. Variable Temperature Magnetic measurement of **1** shows weak anti-ferromagnetism ($\chi_M T$, 9.41cm^{3}Kmol^{-1} at 300 K) with two as good as "isolated" Mn (II) ions (S=5/2 with g ~ 2.07). Magnetic exchange is considered through carboxylato bridged nine/ten atoms inclusive two spanned Mn(II) centres at 4.114 Å. Interestingly, the 3D assembly of **1** exhibits electrical conductivity in the semiconducting region (band gap, 3.72 eV; barrier height, 0.65 eV; series resistance, 0.03Ω). Schottky barrier diode feature is recorded at threshold potential 0.19 V and follows non-Ohmic relation ($I \alpha V^2$) and the conductivity is 3.42×10^{-5}S m^{-1}.

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Development of three novel Schiff base metal Complexes along with their biomedical applications

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Abstract:

By utilizing a piperidine based N, N, O donor Schiff base ligand (HL) [(Z)-4-bromo-2-(((piperidin-2-ylmethyl)imino)methyl)phenol] three novel Cu(II) / Ni(II) complexes $[CuL(N_3)_2(DMF)_2]$ (1), $[NiL(N_3)_2(DMF)_2]$ (2) and, $[Cu(HL)(bpy)ClO_4]$ (3) have been developed and spectroscopically characterized. XRD analysis reveals that complex 1, and 2 are bis μ - azido-bridged binuclear distorted octahedral complexes whereas complex 3 is a mononuclear distorted square pyramidal complex having bipyridyl moiety as an ancillary ligand. All the complexes demonstrate remarkable CT - DNA / HSA protein binding efficacy, confirmed by applying several biophysical studies. The theoretical study in terms of molecular docking supports the experimental findings. The in-vitro MTT assay technique which is done on two cancer cells (HeLa, PA1) and a normal cell (HEK) explores the effective anticancer property of complex 1 and 3 with low toxicity to a normal cell. Nuclear and cellular staining techniques unveil that the complexes can kill the cancer cell via an apoptotic pathway.

Structural interpretation and Photochromic behaviour of azo-based non-transitional metal complexes.

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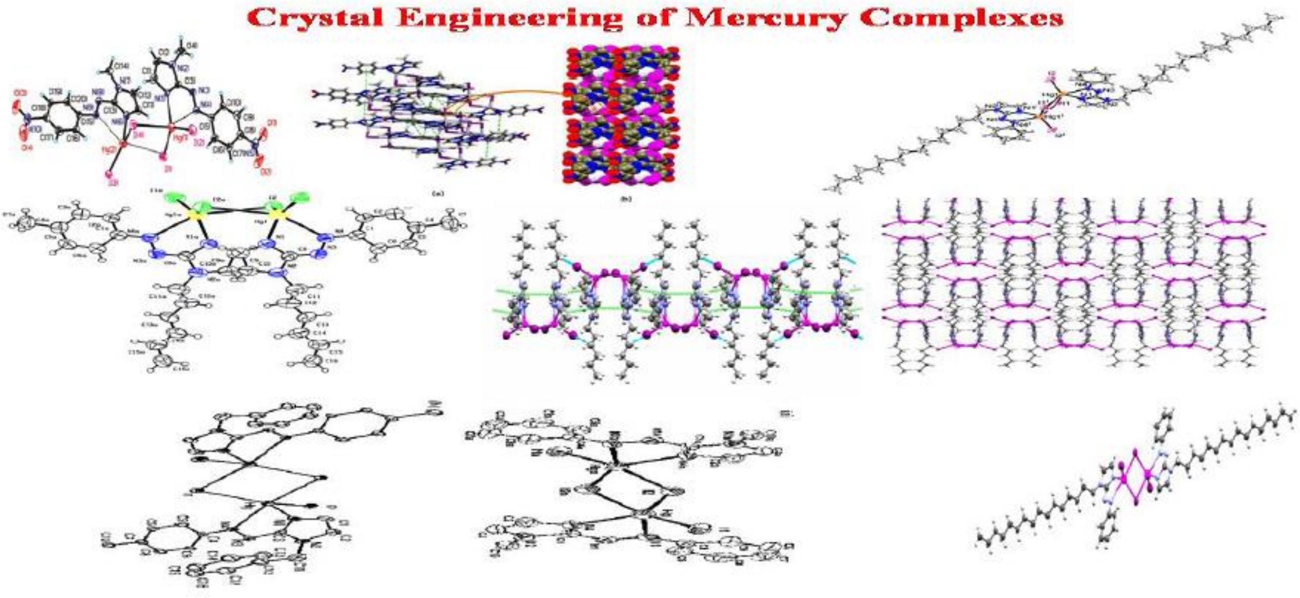
Abstract:

Incorporation of arylazo group to imidazole backbone has synthesized (arylazo)imidazoles. Reaction between some non-transitional metal-halides MX2 (M=Zn(II), Cd(II), Hg(II) and X= Cl, Br, I) and (arylazo)imidazoles (RaaiR/) in MeOH have isolated [M(RaaiR/)2X2] or [M (RaaiR/)(μ-X)(X)]2 depending upon the reaction condition. The structures have been established by spectral (IR, UV-Vis, 1H-NMR) data and the confirmation have been done by single crystal X-ray diffraction studies. UV light irradiation in DMF solution of complexes shows *trans*-to-*cis* (E to Z) isomerisation of coordinated azoimidazole. $(\phi_{t\rightarrow c})$ The reverse transformation, *cis*-to-*trans*, is very slow with visible light irradiation. Quantum yields of *trans*-to-*cis* (E to Z) (E to Z) isomerisation are calculated and free ligand shows higher φ than that of respective complexes. The *cis*-to-*trans* isomerisation is a thermally induced process. The activation energy (E_a) of *cis*-to-*trans* (Z to E) isomerisation is calculated by controlled temperature experiment.



Self-Assembly of a Bis-NHC Ligand and Coinage Metal Ions: Unprecedented Metal Driven Chemistry between the Tri- and Tetranuclear Species

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Abstract:

‘Self-correction’ is an important feature of the self-assembly process, which allows the system to thermodynamically control the formation of a specific architecture over the other possible forms.[1] However, the absence of a clear thermodynamic preference often leads to the existence of several species, occasionally also in equilibrium, in solution. Along this line, we have used a bis-NHC ligand,[2] and we are delighted to report here that the corresponding AgI-NHC complexes exist in equilibrium between the tri- and tetranuclear forms in solution, observed first time for CNHC-donor, which is supported by various studies like NMR (^{1}H, VT, 2D-DOSY), ESI-MS, and concentration studies. It is important to note that this process is exclusive for the AgI-ion in combination with our bis NHC ligand as with other coinage metals (AuI and CuI), no such equilibrium was noticed in the solution. Interestingly, a slow conversion of tetra- to trinuclear form in solution, increases with temp., was observed for the analogous AuI-complexes, whereas the CuI-complexes exist exclusively in tetranuclear form both in solution and solid state.[3]

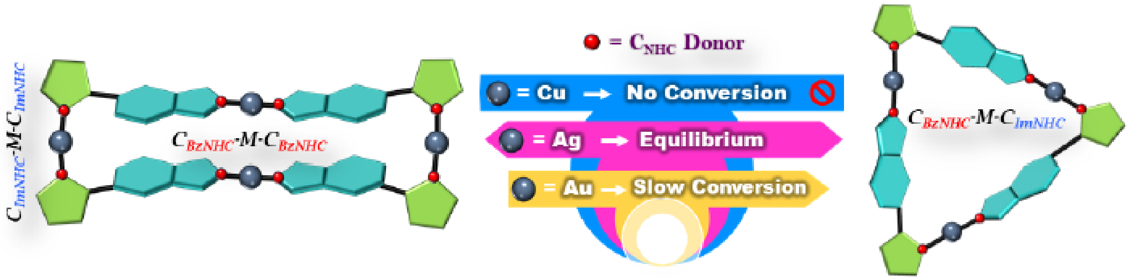

Figure 1. Schematic presentation of the present work.

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Hour-glass and double-decker type conjoined coordination cages

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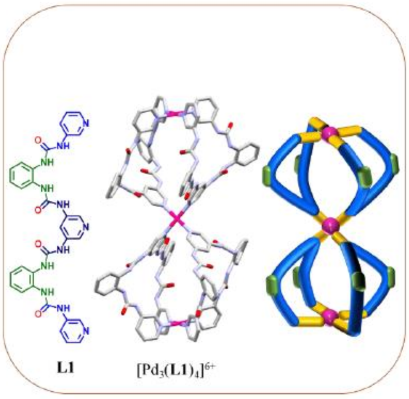
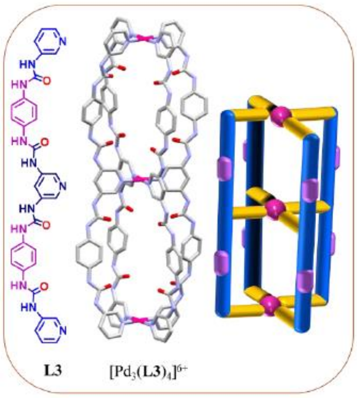
Abstract:

Tailor-made C-shaped bidentate non-chelating ligands have been well utilized for the construction of single cavity PdnL2n type self-assembled discrete cationic cages.1 However, the use of E-shaped/ W-shaped tridentate non-chelating ligands is only sporadically explored. Such ligands (flexible/rigid) afford Pd3L4 type double-decker shaped2 molecules having two cavities. Ligand isomerism in coordination complexes is particularly fascinating as the isomeric complexes are prepared from regioisomeric ligands. In the present work, three regioisomeric tridentate ligands (**L1**, **L2**, and **L3**) are designed and employed to target the preparation of a set of Pd$_3$L$_4$ type, double-decker shaped conjoined-cages ([Pd$_3$(**L1**)$_4$]$^{6+}$, [Pd$_3$(**L2**)$_4$]$^{6+}$, and [Pd$_3$(**L3**)$_4$]$^{6+}$) illustrating ligand isomerism. Interestingly, unprecedented Pd$_3$L$_4$ type, hour-glass shaped conjoined-cages that are isomeric to the double-decker (of the same ligand) are observed in two cases. Double-decker from one ligand and hour-glass from another but regioisomeric ligand exemplifies the ligand isomerism.3 The introduction of flexibility in the backbone of E-shaped ligands could favour hour-glass shaped trinuclear conjoined cages.





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Towards New Coordination Modes of 1,2,3-Triazolylidene: Controlled by the Nature of 1st Metalation in a Heteroditopic Bis-NHC Ligand

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Abstract:

An unusual effect of the nature of first metal coordination of a heteroditopic N-heterocyclic carbene ligand towards the coordination behaviour of 1,2,3-tzNHC is explored. The first metal coordination at the ImNHC site was noted to substantially influence the electronics of the 1,2,3- triazolium moiety leading to an unprecedented chemistry of this MIC donor. Along this line, the Rh^{III}/Ir^{III} -orthometalation in complexes makes the triazolium C4-H more downfield shifted than C5-H, whereas a reverse trend, although to a lesser extent, is observed in case of the non-chelated Pd^{II} -coordination. This difference in behaviour assisted us to achieve the selective activation of triazole C4/C5 positions, not observed before, as supported by the isolation of the homo- and hetero-bimetallic complexes via C5- and C4-metalation, respectively (Figure 1). [1] Further, the %V_{bur} calculation[2,3] eliminates any considerable steric influence and the DFT studies strongly support the selectivity observed during bimetalation.

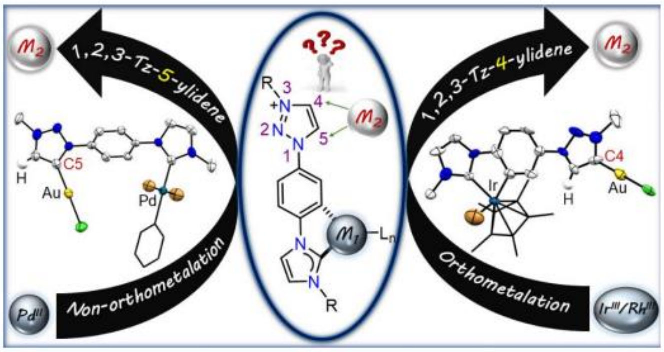

Figure 1. Schematic representation of the present work.

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Iodo bridged lead(II) compounds of azoimidazoles: Synthesis, structure and photochromism

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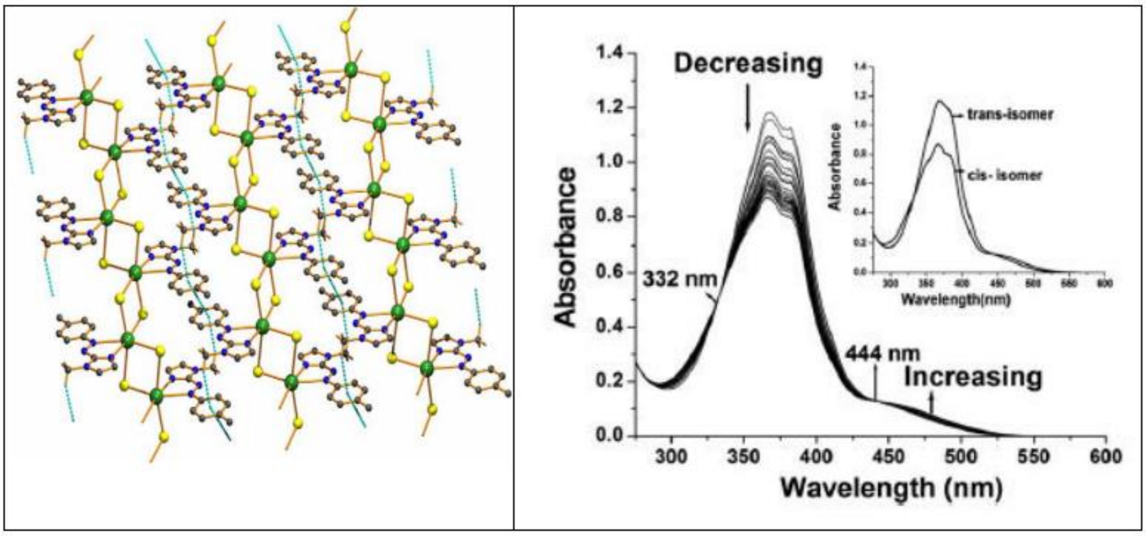
Abstract:

Lead iodide (PbI_2) forms iodo-bridged neutral polymer upon reaction with 1-alkyl-2-(arylazo)imidazoles (RaaiR'). The complexes are characterized by different spectroscopic studies. Structure of iodo-bridged chelated polymer, $[Pb(RaaiR')I_2]_n$, has been established by single crystal X-ray diffraction in one case. The UV light irradiation in DMF solution of the complexes shows E-to-Z (E and Z refer to trans and cis-configuration about –N=N–, respectively) isomerization of the coordinated azoimidazole. Quantum yields and the activation energy (Ea) of the isomerization of the complexes are lower than that of free ligand data.



Suberic Acid as LMWG for achieving bio-active supramolecular metallogels: Efficient anti-pathogenic stuffs against bacterial strains and device-performances of semiconducting diodes

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Abstract:

The article portrays the design, synthesis and significance of three metallogels of suberic Acid instigating Ni (II), Zn (II) and Cd (II) as metal salts. N,N´-Dimethyl formamide has been utilised as a constructing solvent for successive fabrication of all these gel scaffolds. Nickel suberic acid (Ni-SA) metallogel displays finest quality of gelling characteristics among all these synthesised metallogel. Significant variation in microstructural patterns owing to different extent of supramolecular interactions within these soft scaffolds has been observed through FESEM. FT-IR data indicate the remarkable shifting of peaks which might be vitally responsible for the type of various supramolecular interactions involved. These synthesized materials were characterised for their characteristic antibacterial activity. Comparative analysis as an antibacterial agents towards numerous human pathogenic Gram-negative and Gram-positive bacteria were visualised employing spectrophotometer. Investigation on these materials justify them as a promising candidate due to their potential antibacterial activity towards *Klebsiellapneumoniae, Salmonella typhi, Vibrio parahaemolyticus and Gram-positive bacteria Bacillus cereus, Lactobacillus fermentum* and *Staphylococcus aureus*. Along with the biological significances, the synthesized metallogels also show remarkable device-performances of semiconducting diodes. The Current-Voltage characteristics of different metallogels show the Schottky device nature for the gels directed sandwich configuration with ITO/metallogels/Al structure.

Establishment of different aliphatic amines-based rapid self-healing $Mg(OH)_2$ metallogels: Exploring the morphology, rheology, and intriguing Semiconducting Schottky Diode characteristics

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Abstract:

Different aliphatic amines (including triethylamine (TEA), ethylenedimine (EN), N,N,N′,N′-tetramethylethylenediamine (TEMED), diethylenetriamine (DETA), triethylenetetramine (TETA)) directed Mg(II)-metallogels have been successfully achieved. Amines with single or multiple N-site(s) are being utilized for the origination stable Mg(II)-metallogel. The exhaustive rheological investigations establish the mechanical stability of the Mg(II)-metallogels. The thixotropic properties of the rheological experiments clarify the self-healing nature of different Mg(II)-metallogels. The morphological variations of different aliphatic amine directed metallogels are verified through the scanning electronic microscopic images. The presence of metallogel-forming chemicals has been experimentally checked through the elemental analyses. The electrical property of the self-healable Mg(II)-metallogel based systems has been explored. The I-V characteristics of different metallogels show the Schottky device nature for the gels directed sandwich configuration with ITO/metallogels/Al structure. The metallogels mediated fabricated metal-semiconductor junction devices show considerably prominent rectification ratios (on-off ratio).

Photochromism of {μ-Bis(diphenylphosphino)methane}(1-alkyl-2-(arylazo)imidazole) copper(I) perchlorate

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Abstract:

Phosphino bridged dinuclear-Cu(I) complexes, $[Cu(\mu\text{-dppm})(RaaiR/)]_2(ClO_4)_2$ undergoes light induced trans-to-cis isomerization about –N=N– bond. The structures of the complexes have been established by spectral (UV–Vis, IR, 1H NMR) data and the confirmation has been done in case of $[Cu(\mu\text{-dppm})(HaaiEt)]_2(ClO4)_2$ by single crystal X-ray diffraction studies. Optical stimulation using UV light (365 nm) in methanol solution of the complexes shows that the coordinated RaaiR′ undergoes trans-to-cis isomerization about –N=N–Ar. The rate of trans-to-cis isomerization varies 1.11×10^{-8}-1.89×10^{-8} s^{-1} and is largely dependent on mass of the photochrome and strain/steric crowding generated about –N=N– bond. Free ligand shows higher quantum yields ϕ than their complex phase. The cis-to-trans isomerisation is a thermally induced process. The activation energy (Ea) of cis-to-trans isomerisation is calculated by controlled temperature experiment and is found that Ea (ligands) > Ea (complexes).

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Synthesis, Crystal structure, Analysis of Acylpyrazolone based Square pyramidal Cu(II) complexes: *in-vitro* anti-cancer activity on NCI-H23 lung carcinoma cell line.

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Abstract:

Copper complexes have been shown to be effective in cancer treatment due to their cytotoxic action on tumour cells. With the aim of exploring the anticancer properties of coordination compounds, 4-acylpyrazolone based Cu(II) complexes [Cu(HLi)2(DMSO)] (**1**)**,** [Cu(HLii)2(DMF)] **(2),** [Cu(HLiii)2(DMF)] (**3**)**,** has been synthesized and characterized by structural, analytical and spectral methods such as ESI-Mass, FT-IR, UV-Vis, TG-DTA plots, CV, molar conductance and Hirshfeld analysis. The Acylpyrazolone ligand is coordinated to the Cu(II) ion in a neutral fashion as a bidentate ligand. The geometry of these complexes has been determined by single crystal X-ray study, which shows that the geometry of the metal centre is square-pyramidal. The *in vitro* anticancer activity of the complexes was investigated by exposing it to NCI-H23 lung carcinoma cell line using MTT assay. All these results collectively suggest that the complexes could serve as a promising pharmacologically active substance against human lung cancer treatment.

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https://doi.org/10.1016/j.ccr.2019.213069

EFFECT OF DIFFERENT HEATING RATE ON THE THERMAL DECOMPOSITION OF VANILLIN IN AN OPEN REACTION VESSEL

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Abstract:
A study was done of the thermal decomposition of vanillin at different heating rate by thermogravimetric analyzer (TGA). The temperature and enthalpy of fusion of vanillin were calculated based on joint results of the DSC and TG experiments carried out using different heating rates varying from 5 to 150C/min. Thus, it was made possible to compare the contributions to the total thermal effect of vanillin fusion and thermal decomposition process.

Keywords: Thermogravimetric analysis (TGA), heating rate, differential thermal analysis (DTA), DSC, DTG

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2. Mechanistic kinetic analysis of fast pyrolysis of vanillin to primary phenols Attada Yerrayya, Upendra Natarajan and Ravikrishnan Vines Front. *Energy Res.*, **2022**.

Multifunctional sphere-like bimetallic nanoadsorbent $MnAl_2O_4$ (MAO) production in a single pot: a powerful fluoride-removing substance with good elasticity, luminescence, latent fingerprint detection, and magnetic properties

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Abstract:

To remove excess fluoride from water, a spherical-shaped $MnAl_2O_4$ nanoadsorbent was prepared using one-pot synthesis method. By using TGA, XRD, FTIR, Raman, XPS, UV-Visible, FESEM and other techniques, the adsorbent was identified. Batch tests were used to examine the MAO's fluoride adsorption property. The findings demonstrated that the Langmuir isothermal model could accurately describe the fluoride absorption behaviour of the samples, and that the maximum adsorption capacity could be as high as 82% for a 3ppm fluoride solution with an adsorbent dose of 0.15 g/100 mL and a contact period of 30 min. The adsorption kinetics data were properly predicted by the pseudo-second-order models. The regeneration test further demonstrated the sample's great reusability. Additionally, the sample showed good luminescence, latent figure print detection, and magnetic behaviour, making it versatile.

Keywords: Adsorption; Fluoride removal; Adsorption kinetics; Photoluminescence; Magnetism

Syntheses and electrochemical sensing of Cd(II) complexes of N/S containing ligands

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Abstract:

Three new cadmium complexes $[Cd(tht)_2]n$ (**1**), $[Cd(Hpph)_2]n$ (**2**) and $[Cd(mpps)_2]$ (**3**) have been synthesizedwith three different ligands i.e., 2-thiazoline-2-thiol (Htht), N′picolinoylpicolinohydrazide (H_2pph) and potassium N-methylpiperazine-1-carbodithioate (mpps) respectively. These complexes have been characterized by IR, UV-vis., and single X-ray diffraction data. The complexes $[Cd(tht)_2]_n$(**1**), $[Cd(Hpph)_2]_n$ (**2**) and $[Cd(mpps)_2]$(**3**) were crystallized in tetragonal, monoclinic, and triclinic crystal system with space group P 42/n, P21/c, and P-1 respectively. Complexes **1** and **2** are polymeric, while complex **3** is monomeric. Several important interactions were also observed that helps in stabilization of supramolecular architecture of these complexes. The absorption spectrum of complex **2** shows higher λmax as compared to complexes**1** and **3**. The photoluminescence study of complexes shows that complex **2** is relatively more fluorescent than complexes**1** and **3**. The electrochemical behaviour of these metal complexes **1**, **2,** and **3** and sensing of uric Acid (UA) through modified glassy carbon electrodes (GCEs) by these complexes were investigated using cyclic voltammetry. According to the findings, the modified electrode containing complex **3** demonstrated excellent UA electrocatalytic activity. This electrochemical sensing platform for detecting UA has a low detection limit (0.3 μM), good linear ranges (30 to 1500 μM), acceptable sensitivity, and a quick reaction time.

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Design of Inorganic-Organic Hybrid Framework: Synthesis, Characterization and Application.

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Abstract:

A novel Inorganic-Organic hybrid orthorhombic dinuclear Cu(II) Complex [$Cu_2(bpy)_2(4\text{-}Amb)_4(NO_3)(H_2O)_2$] has been synthesized by the reaction of $Cu(NO_3)_3H_2O$ with 4-Amb (4-amino benzoic acid) and Bpy (2,2'bipyridine) through hydrothermal process. The complex has been systematically characterized by elemental analysis, FT-IR, UV, CV, powder X-ray and single-crystal X-ray Crystallography. X-ray single-crystal structural studies indicated that the geometry of the Cu (II) ions is distorted square-pyramidal, where both nitrogen atoms from one bipyridine and two oxygen atoms from two different 4-aminobenzoate ions constitute the square plane and the apical positions are occupied by N-atom of two different 4-aminobenzoate ion.

Keywords: Inorganic-Organic hybrid Framework, Hydrothermal Processes, Cu(II)Complex.

Copper(I)–triphenylphosphine–pyridyl Schiff bases: Synthesis, structural explanation, redox behaviour and DFT computation.

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Abstract:

The reaction of 2-(20-pyridylmethyleneamino)pyridine (L1)/3-(20-pyridyl methyl eneamino) pyridine (L2)/4-(20-pyridylmethyleneamino) pyridine (L3) with CuX (X = Cl, Br, I) and triphenylphosphine (PPh3) affords complexes of composition $[Cu(L)(PPh_3)X]$. These are characterized by microanalytical data and spectroscopic studies (IR, UV–Vis, 1H NMR). The single crystal X-ray structure determines the distorted tetrahedral geometry about Cu(I) in case of $[Cu(L2)(PPh_3)I]$. Cyclic voltammogram shows Cu(II)/Cu(I) couple at 0.5–0.6 V, in addition $[Cu(L)(PPh_3)I]$ shows iodide oxidation peak at 0.3 V. Redox couple negative to SCE may be assigned to the reduction of chelated diimine function. Electronic structure, spectra, emission properties and redox activities are explained by DFT calculations of optimized geometry of $[Cu(L2)(PPh_3)X]$ and have been used to determine the composition and energy of the molecular levels.

Dr. Dibyendu Das

'Life Like Objects' via Systems Chemistry

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Abstract:

There remain critical gaps in our understanding of the emergence of functional biopolymers in the origins of Earth's biosphere. Extant proteins, evolved over millions of years, carry out an impressive array of responsibilities, from catalysis and molecular recognition to motility and compartmentalization. One of the major goals of our lab is to investigate the possible origins of advanced enzymatic functions from folds of short peptide based paracrystalline phases.[1-2] Further, we are excited about understanding the non-equilibrium structures of living systems. I will show our recent discoveries of simple chemical systems that can be substrate-driven to access higher energy self-assembled states, just as seen in natural microtubules. Further, I will attempt to sketch our aims of developing self-assembled autonomous materials that can show temporal control of functions.[3-5]

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5. S. Goswami, A. Reja, S. Pal, A. Singh, and D. Das* *. J. Am. Chem. Soc. 2022 144 accepted article

Dibyendu Das is an Associate Professor in the Department of Chemical Sciences of Indian Institute of Science Education and Research (IISER) Kolkata, West Bengal, India. He received his MSc degree in Organic Chemistry at the University of Calcutta (India) (2005), PhD in Supramolecular Chemistry at Indian Association for the Cultivation of Science (Thesis 2010) and postdoctoral training at the Emory University. From Jan 2017, he is working in IISER Kolkata. Dibyendu leads an interdisciplinary group that focuses on designing active and adaptive materials by harnessing non-equilibrium self-assembly and exploring the functional materials under the purview of systems chemistry. His lab is invested in mimicking how living systems work from the perspective of the emerging and young field of systems chemistry. The intelligence and autonomy of living matter keep inspiring his research to attempt synthetizing materials with adaptive properties.

Awards and Distinctions

1. Featured in "75 under 50 scientists shaping today's India" compendium. On National Science Day, Honorable Minister of State for the Ministry of Science &Technology, Dr Jitendra Singh released this coffee table book published by Vigyan Prasar. The book mentions the profiles of 75 scientists under the age of 50 shaping today’s India.
2. Awarded CRSI Bronze Medal for the year 2023.
3. Awarded Swarnajayanti Fellowship in Chemical Science 2020, DST, Govt of India.(https://dst.gov.in/swarna-jayanti-fellow-develop-intelligent-materials-taking-inspiration-living-matter).
4. Article featured in the virtual issue of the JACS Early Career Investigators as an outstanding work published in 2020.
5. Awarded Indian Peptide Society-Young Scientist Award (IPS-YSA) for excellence in Peptide Research for the year 2021.
6. Awarded CRSI Young Investigator Award 2021 at 27th CRSI National Symposium in Chemistry organized by IISER Kolkata
7. Early Career Advisory Board of ACS Chemical Reviews 2020-2021.
8. Selected as an Associate of the Indian Academy of Sciences (IASc) 2019.
9. Advisory Board of Materials Horizons, 2021.
10. International Advisory Board (IAB) of AsianJOC, 2021 onwards.
11. Awarded INSPIRE Faculty Fellowship from DST, Govt. of India.
12. Articles Featured in the Emerging Investigator Issue Chemical Society Reviews 2022 and Chemical Communications 2020.

Prof. Alakananda Hajra

Design, Synthesis, and Functionalization of Imidazoheterocycles

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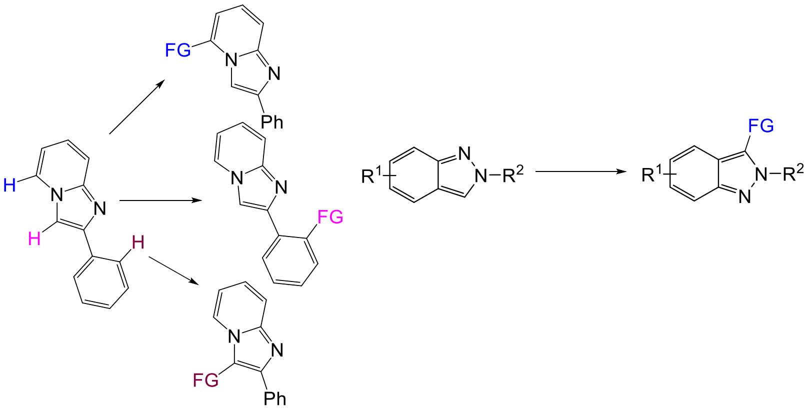
Abstract:

Heterocyclic compounds have gained a great deal of attention as majority of the drugs contain heterocycle scaffolds. So the developments of new synthetic strategies for heterocycles are prime targets of the organic chemists over the years. Imidazopyridine is one of the important fused bicyclic 5–6 heterocycles and it is recognized as "drug prejudice" scaffold due to its wide applications in medicinal chemistry. This scaffold is the constituent of various marketed drug like zolpidem, alpidem, zolimidine, necopidem, saripidem etc. Recently, visible-light photocatalysis has become an impressive tool in organic synthesis. In this realm, the merger of transition metal catalysis and visible light photoredox catalysis offers an exciting opportunity to perform the organic transformations in mild conditions. In this lecture I will discuss our recent works on sustainable synthesis of imidazo[1,2-*a*]pyridines,[1,2] and indazoles[3]



Scheme 1. Regioselective functionalization of imidazopyridine and indazole

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Dr. Alakananda Hajra graduated (M.Sc) from the Department of Chemistry, Indian Institute of Technology, Kharagpur India in 1998. After completing his Ph.D in 2002 under the supervision of Prof. B. C. Ranu from Indian Association for the Cultivation of Science (IACS), Kolkata he joined in SUNY at Albany, USA as a postdoctoral research fellow with Prof. Frank M. Hauser (2002-04). He was also a JSPS research Fellow in the University of Tokyo and worked with Prof. Eiichi Nakamura and Prof. Masaharu Nakamura from November 2004 to May, 2006. He also worked with Prof. N. Yoshikai, NTU, Singapore for one year (2011-2012) as a visiting scientist. His research interests are the development of new synthetic methodologies and green synthetic procedures. He has published more than 190 peer-reviewed articles with more than 8800 citations, giving him a *h*-index of 52.

Awards / Honors / Membership:

- Professor D Nasipuri Memorial Award for the year 2019 by Indian Chemical Society
- Chemical Research Society of India (CRSI) Bronze Medal Award for the year 2018
- Prof. D. K. Banerjee Memorial Lecture Award for the year 2015 from Indian Institute of Science

Prof. Mahiuddin Baidya

Transition Metal Catalyzed C–H Bond Activation Towards Biaryl Frameworks and Natural Product Scaffolds

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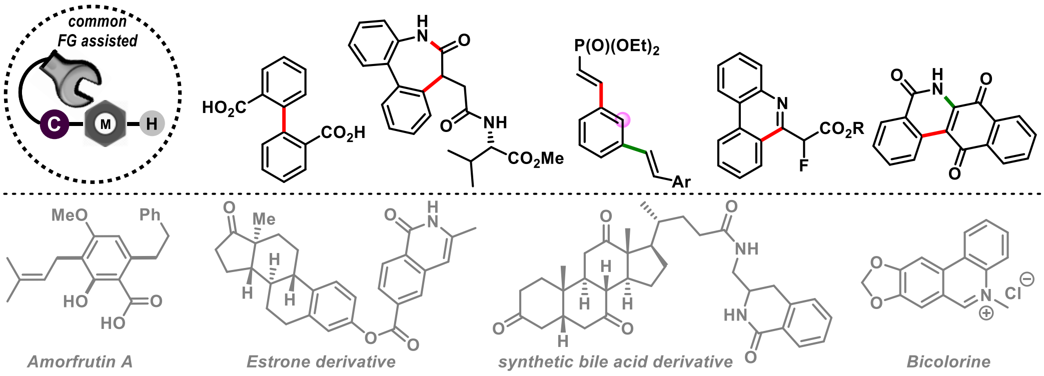
Abstract:

Sustainable synthetic strategies to embrace molecular complexity from simple precursors are fundamental in contemporary organic chemistry. In this context, transition metal-catalyzed functionalization of otherwise inert C–H bonds via exploitation of common organic functional groups (FGs) is highly alluring.[1] In this area, we have delineated the use of carboxylic acid, amide, free-amine, enol, and ketone functionalities as versatile directing groups for a wide variety of position-selective olefination, annulation, and dimerization reactions with versatile ruthenium catalysts.[2] Recently, we have also developed C–H ruthenation step-enabled hydroarylation of alkenes with concomitant decarboxylation *en route* to formal *meta*- and *para*-functionalization and one-pot twofold unsymmetrical olefination of arenes. The developed strategies can be harnessed to synthesize important natural products and late-stage functionalization of bioactive molecules. This presentation will provide an overview of some recent advancements from our laboratory on ruthenium catalysis for C–H bond activation of arenes.



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Mahiuddin Baidya studied chemistry at the Indian Institute of Technology Kanpur (IITK), India. He obtained his PhD in 2009 from Ludwig-Maximilians-Universität München (LMU), Germany under the supervision of Prof. Herbert Mayr. After postdoctoral studies with Prof. Hisashi Yamamoto at The Universality of Chicago, USA and Molecular Catalyst Research Center in Japan with JSPS fellowship, he joined at the Department of Chemistry, Indian Institute of Technology, Madras as an Assistant Professor in 2014 and was promoted to Professor in 2022.

His research interest includes the development of novel concepts on transition-metal catalysis, organocatalysis, and visible-light photocatalysis for organic synthesis, and the synthesis of bioactive natural products and drug candidates.

As an independent researcher at IIT Madras, he has more than sixty research publications in peer-reviewed journals of international repute.

He is a recipient of the INSA-Young Scientist Medal (2017), NASI-Young Scientist Platinum Jubilee Award (2017), Institute Research & Development Award (IRDA IIT M, 2018) and also became an Associate of the Indian Academy of Sciences (IAS) in 2017. Recently, he also received AVRA Young Scientist and Merck Young Scientist Awards.

He served as an Early Career Advisory Board (ECAB) member of *ACS Catalysis* and also is an International Advisory Board Member of *Chemistry – An Asian Journal*.

Prof. Nagendra K. Sharma

Synthesis and Structural Evaluation of Troponyl-Amino Acid/Peptides

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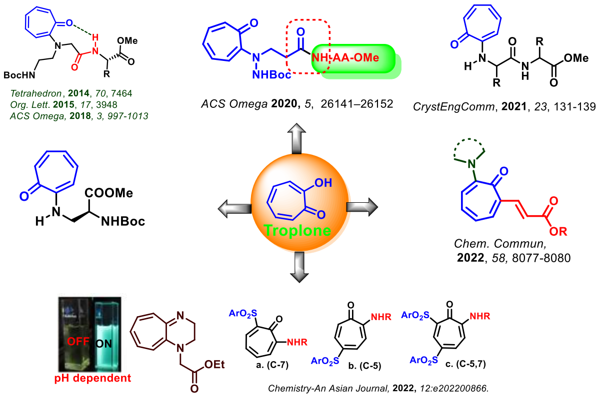
Abstract:

Tropolone is a no benzenoid aromatic molecule, which is a constituent of *troponoid* natural products.[1] It is a natural scaffold to form a complex with coordinating metal ions. Their natural and synthetic derivatives are inhibitors of various metal-dependent enzymes and are considered promising therapeutic drug candidates.[2, 3] Importantly, troponyl derivatives exhibit unique photophysical properties along with fluorescence owing to the π-π*, n-π*, and charge transfer though the quantum yield of Tropolone is low.[4, 5] Recently, we have introduced troponyl scaffold into rationally designed amino acids for tunning the structural and functional properties of peptides. Troponyl residue of *troponyl*-peptides play significant role in the structural and conformational changes which provide an opportunity to design an novel chromophoric peptidomimetics.



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Prof. Nagendra K. Sharma received Ph.D. (Chemistry) award (2006) from premier research institute of CSIR, National Chemical Laboratory (NCL)-Pune and University of Pune, Pune (India) under the supervision of Prof. Krishna N. Ganesh. He was involved in the chemical synthesis of nucleic acid analogue, Peptide Nucleic Acid (PNA) and related molecules and demonstrated their comparative biophysical studies with DNA/RNA. He did postdoctoral research as NIH-postdoctoral fellow (2006-2009) under the guidance of Prof. Dale C. Poulter, University of Utah-Salt Lake City, Utah (USA). He was involved in the syntheses of various substrate/inhibitors of isoprenoid IPP isomerases enzymes (IDI-1 & IDI-2) and shown the reaction mechanism of IPP-DMAPP isomerization. Currently he is associate professor at NISER-Bhubaneswar and involved in the teaching and fundamental research in the area of organic chemistry/Bioorganic Chemistry. He is very keen to explore the peptides-Nucleic acid interactions in the central dogma of biology (Replication/Transcription/Translation). His research laboratory mainly comprises the synthesis of modified amino acids/peptides and DNA/RNA analogues to improve biochemical properties of native ones which are in demands for the development of new therapeutic drug candidates. His group has established the synthesis of unnatural amino acids/peptides via C-H activation for new peptides foldamers. Now his laboratory is capable for the chemical/enzymatic syntheses of conjugated DNA/RNA analogues. Recently he has started the synthesis of modify CRISPR analogues to improve the nuclease activity of CRISP-Cas9 complex with specific DNA duplex *in vitro*/*in vivo* conditions.

Prof. Manmohan Kapur

New Pathways in Indole Synthesis by Applying TM-Catalyzed C-H Functionalization

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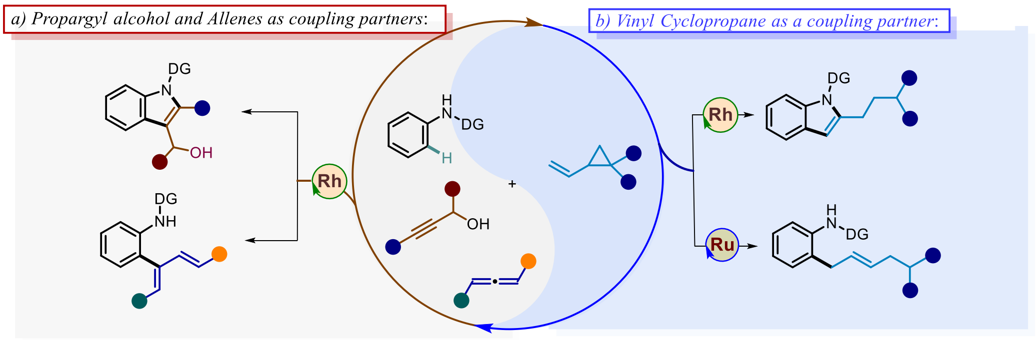
Abstract:

Organic transformations promoted by TM-catalysis have presented a new platform in designing innovative routes for atom- & step-economical synthesis of diverse heterocyclic scaffolds.[1] As a class of *N*-containing heteroaromatics, substituted indoles are one of the most abundant and important heterocycles in the natural world and form the core of numerous biologically active compounds.[2] In this regard, electronically unbiased allenes, their preformed synthetic precursors *i.e.*, propargyl alcohols and vinyl cyclopropanes have gained increasing attention of the synthetic community owing to their diverse reactivity patterns. We have used these reactive coupling partners for synthesizing diverse indole skeletons by tuning their reactivity patterns. The transformations encompass extensive substrate compatibility along with detailed mechanistic studies to validate the efficiency of the methodologies. Not only that, interesting synthetic transformations of the products also lead to the construction of synthetically useful molecular frameworks which are otherwise difficult to achieve and enhances the overall viability of the methodologies.[3]



Scheme 1: New pathways in indole synthesis

References:

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Manmohan Kapur received his Ph.D. degree in 2003, working under the supervision of Prof. Ganesh Pandey at National Chemical Laboratory, Pune. In the same year, he joined the group of Prof. Jin K. Cha at the Wayne State University, Detroit, USA, as a postdoctoral fellow. In 2004, he was awarded the Alexander von Humboldt Postdoctoral Research Fellowship for his second postdoctoral position at the Institut für Organische Chemie, Universität Tübingen, Germany, under the guidance of Prof. Dr. Martin E. Maier. Upon his return to India, he joined the industry before moving to Indian Institute of Science Education and Research Bhopal in 2009, where is presently a Professor in the Department of Chemistry. His research interests include the total synthesis of natural products by employing transition-metal catalysis as the key step and synthesis of natural products bearing peptide-based backbones, especially certain classes of anti-mycobacterial agents. He is the recipient of the Bronze Medal of the Chemical Research Society of India (CRSI) (2020) and the SERB-STAR Award (2020), Golden Jubilee Visiting Fellowship of ICT Mumbai (2021-22). He is also the member of the International Advisory Board of the *Asian Journal of Organic Chemistry*.

Dr. Suman De Sarkar

Controlling Radical Reactivity under Photo- and Electro-chemical Coditions

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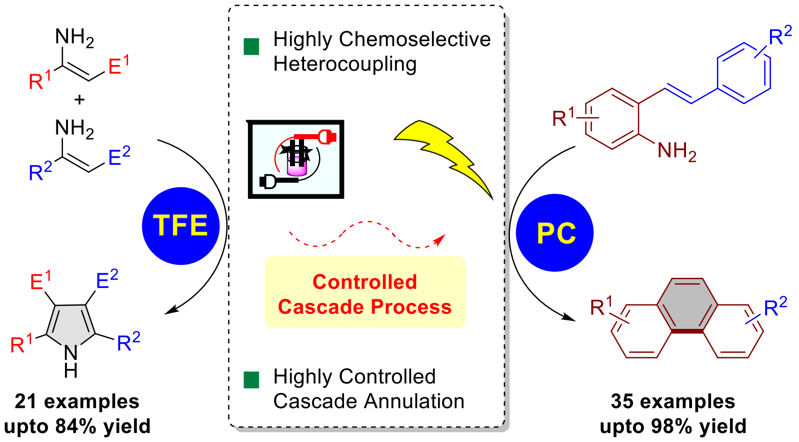
Abstract:

Radical transformations are undoubtedly one of the most powerful tools in Organic Synthesis.[1] However, controlling the reactivity of the short-lived radicals is a major challenge to organic chemists. Herein, we present an electrochemical strategy for the efficient heterocoupling of aryl- and alkyl-substituted enamines to synthesize tetrasubstituted NH-pyrroles by controlling the reactivity of *in situ* generated radicals.[2] In another work, an efficient approach for the synthesis of phenanthrene scaffolds by utilizing the dual catalytic activity of an organo-photocatalyst is presented.[3] The controlled cascade transformation proceeds via *in situ* diazotization followed by olefin isomerization and subsequent arene radical generation through photoreduction.



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3. Mandal, T.; Mallick, S.; Kumari, N.; De Sarkar, S. *Org. Lett.* **2022**, *24*, 8452.

Suman De Sarkar received B.Sc. (2005) and M.Sc. (2007) degrees in Chemistry from University of Calcutta and Indian Institute of Technology Kanpur, respectively. He obtained his Ph.D. in November 2010 from Westfälische Wilhelms University Muenster under the supervision of Prof. Armido Studer. Afterward, he worked as a postdoctoral researcher in the research group of Prof. Karl Gademann at the University of Basel (2011 to 2013) and with Prof. Lutz Ackermann as an Alexander von Humboldt Postdoctoral Fellow at the University of Goettingen (2013 to 2015). In October 2015 he joined Indian Institute of Science Education and Research Kolkata, India, as an Assistant Professor and in September 2019 was promoted to the post of Associate Professor. His research focuses on the application of redox-mediated transformations in organic synthesis with special interests in electrochemistry and photo redox catalysis.

Prof. Akhilesh Kumar Verma

Construction of Biologically Important Small Organic Molecules from Alkynes

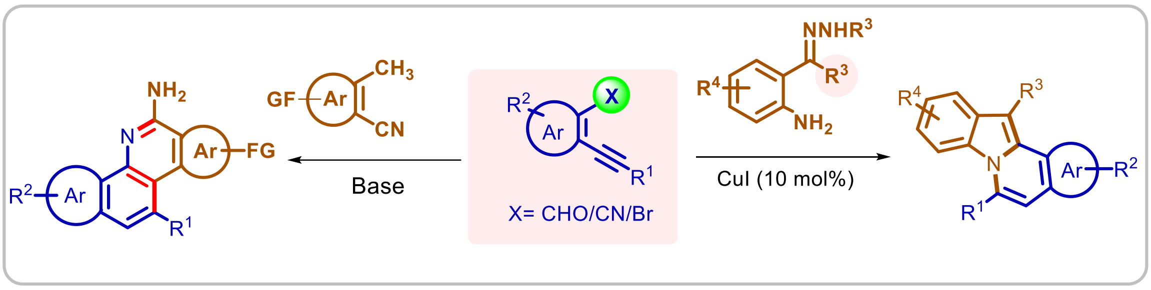
Akhilesh Kumar Verma*

Department of Chemistry, University of Delhi

Email: *averma@acbr.du.ac.in*

Abstract:

The simplicity, efficiency, and generality of reactions using alkynes have led to their applications in the synthesis of a wide variety of small organic molecules and natural products. Developing synthetic strategies for small molecules in terms of selectivity, operational simplicity, functional group tolerance, and environmental sustainability is in constant demand as the majority of drugs; drug-like compounds contain hetero atoms at their core. In continuation of our interest in the synthesis of small organic molecules using alkynes chemistry, we have successfully engineered the synthesis of a variety of biologically important scaffolds using hydroamination/electrophilic cyclization/annulation of alkyne chemistry.[3] In this presentation I would like to discuss some recent results in this chemistry.



References:

[1] Akhilesh K. Verma*, T. Kesharwani, J. Singh, V. Tandon, R. C. Larock***** *Angew. Chem. Int. Ed*. **2009**, *48*, 1138
[2] Monika Patel, Rakesh K. Saunthwal and Akhilesh K. Verma* *Acc. Chem. Res*. **2017**, *50*, 240
[3] Akhilesh K. Verma* Megha Joshi and Ved Prakash Singh *Org. Lett.* **2011**, *13*, 1630
[4] Megha Joshi, Rakesh K. Tiwari, and Akhilesh K. Verma* *Org. Lett*. **2012**, *14*, 1106
[5] Megha Joshi, Monika Patel, Rakesh Tiwari, Akhilesh K. Verma******J. Org. Chem*. **2012**, 77, 5633.

[6] Akhilesh K. Verma,* Rajeev R. Jha, Ritu Chaudhary, Rakesh K. Tiwari, Kotla Siva K. Reddy, and Abhinandan Danodia *J. Org. Chem*. **2012**, *77*, 8191

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[8] Akhilesh K. Verma**,*** Abhinandan K. Danodia, Rakesh K. Saunthwal, Monika Patel, and Deepak Choudhary *Org. Lett*. **2015,** *17*, 3658
[9] Pawan K. Mishra, Shalini Verma, Manoj Kumar, and Akhilesh K. Verma* *Org. Lett*. **2018,** *20*, 7182

[10] Manjusha V. Karkhelikar, Rajeev R. Jha, B. Sridhar, Pravin R. Likhar* and Akhilesh K. Verma* *Chem. Commun.* **2014,** *50,* 8526-8528
[11] Shalini Verma, Manoj Kumar, and Akhilesh K. Verma* *Org. Lett.* **2020**, *22*, 130

Brief-Biodata

Prof. Verma received his Ph.D. degree from the Department of Chemistry, University of Delhi. He joined Dr. B. R. Ambedkar Center for Biomedical Research, University of Delhi, as a Lecturer on 2nd Feb 1998 and later moved to the Department of Chemistry as a Reader on 23rd Jan 2009; he was promoted to Associate Professor in 2010 and became full Professor in 2013. He also served School of Physical Sciences, JNU for nearly one year (2015). He did his postdoctoral research work from 2001 to 2002 (two years) with Prof. Alan R. Katritzky at the University of Florida USA, and also worked as visiting Scientist from 28th June 2007 to 31st August 2008 at Iowa State University of Science and Technology, Ames, Iowa, USA in the Laboratory of Prof. Richard C. Larock. Prof. Verma has guided 38 Ph.D. students and published more than 138 research papers (*h*-Index:42, I-index: 94; Citation: 5611).

Research Interests:

- Theme One (Basic): (i) Design and Synthesis of new molecular entities for drug development in a sustainable manner (ii) Mechanistic investigation of organic reactions by capturing fleeting intermediates using the online mass-spectrometry technique.
- Theme two (Applied): Metal-free and cost-effective method for the deuteration of N, O, and S-heterocycles/carbocycles

Awards and Honours (Selected):

- **2021:** Elected Fellow (FNA), Indian National Science Academy (INSA)
- **2021:** Bronze Medal, Chemical Research Society of India (CRSI)
- **2021:** Elected Fellow Royal Society of Chemistry (FRSC)
- **2021:** Senior Fellow, Institution of Eminence (IoE); University of Delhi
- **2019:** Member Governing Body, CCRUM, Ministry of AYUSH
- **2017:** UGC Mid-Career Award
- **2007:** BOYSCAST Fellow (2007-2008)

Positions Held:

- Professor: Department of Chemistry, Univ. of Delhi (March 2013-till date)
- Professor: School of Physical Sciences, JNU (Jan.2015 to Nov. 2015 On Lien)
- Associate Professor: Depart. of Chemistry, Univ. of Delhi (Jan 2009 to March 2013)
- Assistant Professor: ACBR University of Delhi (Feb. 1998 to Jan. 2009)

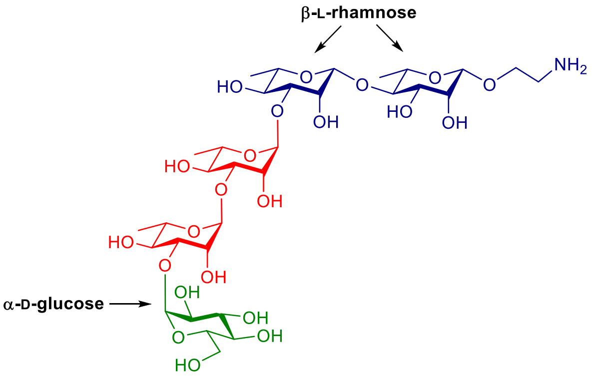
Prof. Balaram Mukhopadhyay

Carbohydrates: The Sweet World

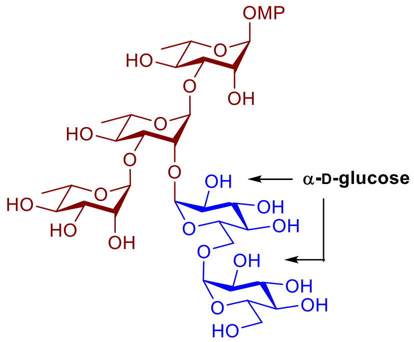
Balaram Mukhopadhyay
Professor, Sweet Lab, Department of Chemical Sciences
Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur *sugarnet73@hotmail.com*, *mbalaram@iiserkol.ac.in*

Abstract:

Unicellular bacteria are continuously intriguing us with newer complex oligosaccharides that are posing challenges for the synthetic carbohydrate chemists for their chemical synthesis. The potential of O-antigen repeating units towards the development of synthetic/semi-synthetic vaccines continues to attract synthetic chemists to formulate accurate and scalable synthetic protocols to get these complex oligosaccharides in the purest possible form. The presentation will elaborate the detailed synthetic protocol *en route* to the pentasaccharide repeating units from *Halomonas ventosae* RU5S2EL and *Ruminococcus gnavus*. The associated stereo- and regioselectivity challenges will be discussed in detail.



Pentasaccharide repeating unit from *Halomonas ventosae* RU5S2EL



Pentasaccharide repeating unit from *Ruminococcus gnavus*

In addition to our efforts towards the total synthesis of bacterial oligosaccharides, we are trying to use carbohydrate multivalency to develop biomarkers, looking at the possibilities of developing multifunctional small molecule carbohydrate materials and exploring the mechanical properties of carbohydrate crystals. These aspects will be touched upon briefly during the presentation.

Reference:

- D. Pal, M. Naskar, A. Bera and B. Mukhopadhyay, *Carbohydr. Res.* **2021**, *507*, 108384.
- D. Pal and B. Mukhopadhyay, *J. Org. Chem.* **2021**, *86*, 8683-8694.
- R. Das and B. Mukhopadhyay, *Tetrahedron Lett.* **2016**, *57*, 1775-1781.
- M. K. Panda, K. B. Pal, G. Raj, R. Jana, T. Moriwaki, G. D. Mukherjee, B. Mukhopadhyay and P. Naumov, Cryst. Growth Des. **2017**, *17*, 1759-1765.
- K. B. Pal and B. Mukhopadhyay, *ChemistrySelect* **2017**, *2*, 967-974.
- S. Mukherjee, G. R. Krishna, B. Mukhopadhyay, C. M. Reddy, *Cryst. Eng. Comm.* **2015**, *17*, 3345 - 3353.
- S. Mukherjee and B. Mukhopadhyay *RSC Adv.* **2012**, *2*, 2270 - 2273.

Details of professional training and research experience:

Doctor of Philosophy

Mar 1997- Sep 2001; Department of Biological Chemistry, Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700 032. Chemical synthesis of biologically important carbohydrate molecules and development of new methodologies for the synthesis of mono- and disaccharide building blocks.

Senior Postdoctoral Research Associate

Sep 2001-Sep 2005, Centre for Carbohydrate Chemistry, School of Chemical

Sciences and Pharmacy, University of East Anglia, Norwich NR4 7TJ, UK.

Chemical and enzymatic synthesis of biologically active oligosaccharides, synthesis

and evaluation of carbohydrate modified gold nanoparticles and glyco-quantum dots.

Details of employment:

Scientist C

Sep 2005-Dec 2007: Medicinal and Process Chemistry Division, Central Drug

Research Institute, Lucknow

Assistant Professor

Jan 2008-Dec 2012: Department of Chemical Sciences, Indian Institute of Science

Education and Research (IISER) Kolkata

Associate Professor

Dec 2012-Oct 2018: Department of Chemical Sciences, Indian Institute of Science

Education and Research (IISER) Kolkata

Professor

Oct 2018-Till date: Department of Chemical Sciences, Indian Institute of Science

Education and Research (IISER) Kolkata

Other Details

1 Total number of PhD awarded: 14

2 Total number of MS Thesis: 8

3 Number of Current Students: 7

4 Number of Papers published in International Journals: 112

5 Number of Book Chapters :3

6 Number of Patent: 1

7 Number of Extramural Projects (DST, CSIR, Swedish Research Council, SERB): 6

Dr. Rajarshi Samanta

Migratory Insertion of Quinoid Carbene: Useful Tool for Step-Economic Construction of Azaheterocycles

*Rajarshi Samanta**

Department of Chemistry

Indian Institute of Technology Kharagpur Kharagpur 721302

***(Email:** rsamanta@chem.iitkgp.ac.in)*

Abstract:

The diazo quinone or quinone diazide compounds have been extensively utilized to introduce phenol/naphthol moieties into hydrocarbons or nitrogen-containing heterocycles under transition metal catalysis. The reactions proceed via C–H insertion or migratory insertion of metal carbenes.[1] Due to site-selectivity issues, directed C–H metalation, metal–quinoid carbene formation followed by migratory insertion has achieved considerable attention.[2] In this presentation, regioselective arylation of quinoline scaffolds to provide 8-azaBINOL based on the migratory insertion of quinoid carbenes will be discussed.[3] Further, the racemic synthesis of important phosphine ligands like QUINAP, METHOX, PINAP, PHENAP will be discussed.[4] Construction of indolocoumarin using this strategy will also be explained.[5] Finally, a mild *N*-arylation using a similar strategy will also be presented.[6]

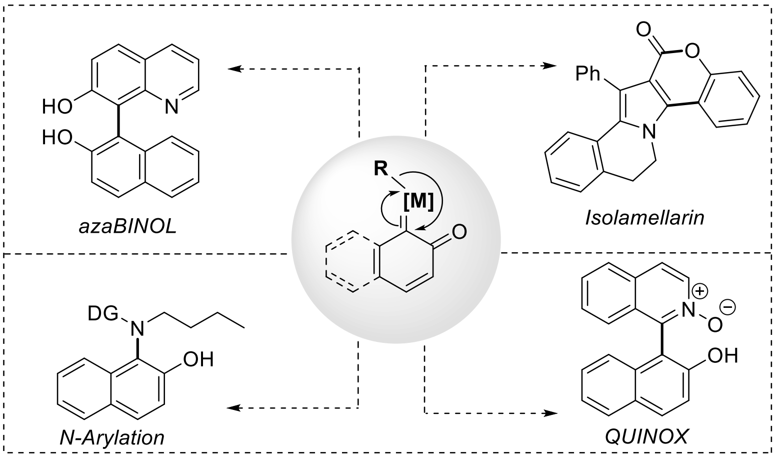


Figure. Migratory insertion of quinoid carbene for the site-selective arylation

References and Notes:

1. Hu, F.; Xia, Y.; Ma, C.; Zhang, Y.; Wang, J. *Chem. Commun.* **2015**, *51*, 7986-7995.
2. Bera, S.; Sarkar, S.; Samanta, R. *New J. Chem.* **2021**, *45*, 10135-10149.
3. Ghosh, B.; Biswas, A.; Chakraborty, S.; Samanta, R. *Chem Asian J* **2018**, *13*, 2388-2392.
4. Biswas, A.; Pan, S.; Samanta, R. *Org. Lett.* **2022**, *24*, 1631-1636.

5. Sarkar, S.; Samanta, R. *Org. Lett*. **2022**, *24*, 4536-4541.

Brief-Biodata

Rajarshi Samanta did his bachelor's (2002) and master's (2004) from Jadavpur University. He received his PhD from the Indian Institute of Chemical Technology, Hyderabad in 2010 under the supervision of Prof. Tushar Kanti Chakraborty. Subsequently, he moved to Max Planck Institute, Dortmund, Germany for his postdoctoral work under Prof. Andrey P Antonchick as Max-Planck postdoctoral researcher. Then he joined at Indian Institute of Technology, Kharagpur as an assistant professor in September 2013 and was successively promoted to associate professor in August 2019. He received Associateship for the Indian Academy of Sciences (2019-2022) and was selected as an Emerging Investigator, *New Journal of Chemistry* (2021).

Current Research Interest:

- Development of transition metal-catalysed step economic transformations especially using diazo compounds via the formation of metallocarbenes/nitrenes.
- Synthesis of bioactive natural products using the developed methods.
- Direct late-stage modifications of various complex heterocyclic molecules in a catalytic way.
- Development of step-economic methods for the construction of heteroatom-containing organic extended π-conjugated systems and screening their activity in biological assays as well as organic material.

Prof. Dipankar Srimani

Sustainable Transformations of Alcohols Using Acceptorless Dehydrogenation and Borrowing Hydrogen Catalysis

Dipankar Srimani

Department of Chemistry, Indian Institute of Technology-Guwahati,

Kamrup, Assam 781039, India.

***E-mail:** dsrimani@iitg.ac.in*

Abstract:

Consumption of fossil fuels has increased significantly over the last half-century, which has led to rapid fossil fuel depletion. This creates an increasing demand for developing new valuable compounds using renewable starting materials. In this perspective, chemicals derived from lignocellulose biomass can set the best example. As alcohols can be easily produced from lignocellulosic biomass, it is worthwhile to use renewable alcohols for various chemical transformations using a waste-free process. Acceptorless Dehydrogenation (AD) and Borrowing Hydrogen (BH) catalysis are two extremely powerful strategies that can directly utilize the alcohols for the production of various fine chemicals via C-C and C-heteroatom bond-forming reactions.[1] Instead of releasing toxic chemical wastes, the major advantage of the AD and BH catalysis is that it either can release dihydrogen molecules or utilizes the dihydrogen molecules via transfer-hydrogenation.

We have recently developed new air-stable ruthenium and earth-abundant manganese-based catalysts and explored their activity toward different AD coupling reaction BH catalysis. [2] The scope and limitation of these catalysts towards the synthesis and functionalization of various heterocycles have been investigated. The lecture will cover the fundamental concepts of AD and BH catalysis and the details of these works.

References:

1. For review see: (a) A. Corma, J. Navas and M. J. Sabater, Chem. Rev. 2018, 118, 1410−1459.

2. (a) K. Das, A. Mondal and D. Srimani, J. Org. Chem. 2018, 83, 9553-9560; (b) K. Das, A. Mondal and D. Srimani, Chem. Commun., 2018, 54, 10582-1058; (c) K. Das, A. Mondal, D. Pal and D. Srimani, Org. Lett. 2019, 9, 3223-3227.

Dipankar Srimani received his PhD (2011) from IACS, Kolkata under the supervision of Prof Amitabha Sarkar. He pursued his post-doctoral research (2011–2014) at Weizmann Institute of Science with Prof. David Milstein. In 2015, he joined the DST-INSPIRE faculty at IIT-ISM Dhanbad. In the same year, he moved to the Indian Institute of Technology-Guwahati and joined the Dept. of Chemistry as an Assistant Professor. Since 2019 he has been an Associate Professor at IIT-Guwahati. His research mainly focuses on the development of air-stable earth-abundant transition metal complexes and metal doped supported materials for catalytic applications.

Dr. Nanda D. Paul

Exploring Applications of Well-Defined Transition Metal Complexes of Redox-Noninnocent Ligands: From Catalysis to Molecular Electronics

Dr. Nanda D. Paul
Department of Chemistry
Indian Institute of Engineering Science and Technology, Shibpur
Botanic Garden, Howrah 711103, India
Email: *ndpaul@gmail.com; ndpaul2014@chem.iiests.ac.in*

Abstract:

The chemistry of transition metal complexes of redox-noninnocent ligands has gained immense attention over the years because of its interesting electronic structures. Over the decades, the primary research in this area was focused on understanding the ambiguous electronic structure and bonding of such complexes. Only in the last decade it has shifted more to catalysis and, very recently, towards more physical applications upon realizing the fact that redox-noninnocent ligands, other than coordinating metal ions and offering steric control, can participate synergistically with the metal ions during electron transfer events and influence a chemical transformation in many ways.

This lecture will be focused on the plausible application of a few well-defined transition metal complexes of some chosen redox-noninnocent ligands in homogeneous catalysis and molecular electronics. A few examples will be discussed, how multi-electron chemical transformations and radical-type reactions can be achieved using 3d-metal-catalysts, avoiding thermodynamically unfavorable metal-centered redox events. Plausible applications of transition metal complexes in molecular electronics will also be highlighted.

References:

(1) Sikari, R.; Sinha, S.; Chakraborty, G.; Das, S.; van Leest, N. P.; Paul, N. D.* *Adv. Synth. Catal.* **2019**, *361*, 4342–4353.

(2) Das, S.; Mondal, R.; Chakraborty, G.; Guin, A. K.; Das, A.; Paul, N. D.* *ACS Catal.* **2021**, *11*, 7498−7512.

(3) Mondal, R.; Guin, A. K.; Pal, S.; Mondal, S.; Paul, N. D.* *Org. Chem. Front.* **2022**, https://doi.org/10.1039/D2QO01196D.

(4) Sinha, S.; Sahad E, M.; Mondal, R.; Das, S.; Manamel, L. T.; Brandão, P.; Bruin, B. de.; Das, B. C.; Paul, N. D.* *J. Am. Chem. Soc.* **2022**, DOI: https://doi.org/10.1021/jacs.2c08941.

Dr. Nanda Dulal Paul, originally from Kamakhyaguri, after completing his schooling from Kamakhyaguri High School, passed B. Sc, with Chemistry (Hons.) from St. Xaviers College, Kolkata in 2005 and completed his M.Sc. in chemistry with Inorganic Chemistry specialization in 2007 from the University of Calcutta. He did his Ph.D. at the Department of Inorganic Chemistry, IACS, Kolkata under the supervision of Professor Sreebrata Goswami from 2007-2012. In July 2012 he moved to the van't Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands as an ERC funded scientific researcher. Before completing his tenure as a scientific researcher at HIMS with Prof. Bas de Bruin, he was offered the position of Assistant Professor at the Department of Chemistry, IIEST, Shibpur in November 2013. Since January 2014, he is an Assistant Professor at the Department of Chemistry, IIEST. He is married to Sutanuva and has two little sons Navayan and Suvayan.

Dr. Mandar Bodas

Development of NCE as Inhibitor of Rock Kinase for Heart Failure

Dr Mandar Bodas, Solution Consultant Elsevier

Abstract:

Rho-associated protein kinases (ROCK1 and ROCK2) belong to the AGC family of serine-threonine kinases and regulate a wide range of fundamental cell functions. Inhibition of ROCK has been proven to be of potential therapeutic benefit for a variety of diseases. Rho kinases (ROCKs) are the most extensively studied effectors of the small G-protein RhoA and abnormalities in RhoA/ROCK signalling have been observed in various cardiovascular diseases. The ROCK pathway is a key player in different smooth muscle cell functions including contractility, proliferation, and migration. The NCE developed was able to differentiate ROCK2 selectivity over ROCK1 and demonstrated target engagement with excellent kinase selectivity, whole blood potency, no changes in blood pressure and heart rate in mouse telemetry.

Dr. Amit Kumar

Decoding the Chemistry of Primary Amide/Imidates for Functionalization Reactions

*Amit Kumar**

Department of Chemistry

Indian Institute of Technology Patna, Bihar, India

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

Abstract:

Functionalized organic molecules are an important class of compounds that are ubiquitously present as a key structural motif in natural products, and biologically active compounds. The introduction of the required functional motif into the desired system with satisfying the parameters of sustainable chemistry such as cost and atom economy is high in demand. Therefore, the direct functionalization of robust and unreactive C-H (sp^2/sp^3) bonds provides an alternate, effective, and desirable tool to organic chemists to convert them into valuable chemical commodities.[1] However, major challenges lies with these methods regio- and chemo-selective functionalization of C-H bonds. To overcome these issues, the concept of directing group was introduced, which offers chemoselective transformations.

Hence, in the past decade, a variety of DGs have been introduced for regioselective C-H transformation. In general, these strategies required the preinstallation of directing groups followed by their uninstallation, which demands two extra steps, resulting in the eventual reduction in the atom and step economy of the complete transformation. Despite the ubiquitous presence of primary amide/imidates functionality, has been rarely utilized as a DGs owing to its least reactive nature and makes an unattractive and challenging synthon. Considering the high abundance and challenges, we became interested in exploring the chemistry of primary amide/Imidates as optimal directing groups for the synthesis of high value-added derivatives of organic compounds.[2] The scope and limitations of such chemistry will be discussed using selected examples.

References:

1. Lyons, T.W.; Sanford, M. S. *Chem. Rev*. **2010**, *110*, 1147.

2. (a) Y. Kumar, Y. Jaiswal and A. Kumar *Org.Lett.*_**2018**,*20*,4964. (b) **Kumar, Y.,** Jaiswal, Y., Kumar, A. *J. Org. Chem.* **2016**, *81*, 12247. **(c) Kumar, Y.,** Shaw, M., Thakur, R., Kumar A. *J. Org. Chem.* **2016**, *81*, 6617

Career profile:

- Associate Professor, IIT Patna **5th Dec. 2019**
- Assistant Professor, IIT Patna: **2014-4th Dec. 2019**
- Research Investigator-Biocon-Bristol Myers Research Center,
- Postdoctoral Fellow-University of Konstanz, Germany: **2010-**
- Postdoctoral Fellow -City University of New York, USA: **200**
- Ph. D. IIT Kanpur, India: **2008**
- M. Sc. Delhi University: **2002**

Honours and awards:

- CRSI-Bronze medal award **2023**
- Life-member- CRSI, India
- Life-member-ISCB, India
- Life-member, ACIIT, India

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

Representative Publications:

1. *Chem.Commun.* **2022**, *article in press*
2. *J. Org. Chem.* **2021**, *86, 9744*
3. *Org. Letter,* **2020**, *22, 5, 1908*
4. *Org. Letter,* **2020**, *22,4,1605*
5. *Org.Lett.* **2018**, *20, 4964*
6. *Org.Lett.*_**2018**,*20,4964*
7. *Chem.Commun.* **2018**, *57, 7207*
8. *J. Org. Chem.* **2018**, *83*, 12247
9. *J. Org. Chem.* **2016**, *81*, 6617

Dr. Ashoke Sharon

Structure, Computation, and Chemistry for HSP90: A target protein exploration for Drug Discovery

Ashoke Sharon

Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India.

Email ID: *asharon@bitmesra.ac.in*

Abstract:

Heat shock protein 90 (Hsp90), a host chaperone protein system, controls the NF-κB pathways to reactivate the viral reservoir from latency. HSP90 also induces viral gene expression and HIV-1 reactivation by CD4$^+$ T-cell activation. This is the main reason that HIV-1 reactivation is a global health concern and cannot be handled by applying existing drugs, including cART, which overall does not provide a complete cure for HIV. Thus, to achieve a functional treatment against HIV, targeting host factors such as HSP90 is one promising strategy. Our research group is involved in the exploration to understand the facets of HSP90 towards the discovery of new molecules as potential antiviral

Hsp90 worked through its structural flexibility to bind with co-chaperones and client proteins to mediate biological function. The co-chaperone, Cdc37, binds to the Cdk4 client protein and stabilizes the Hsp90-Cdc37-Cdk4 protein complex. Further, the destabilizing protein-protein complex may prevent the requisite folding of the misfolded conformation of Cdk4. Studying the protein-protein interface, followed by designing a suitable ligand or drug, is challenging. However, it may give a direction to discover a therapeutic molecule to alter protein-protein interaction. To achieve this, the protein complex is computationally investigated using several simulation techniques to delineate the protein-ligand & protein-protein interaction portfolio and the possibility of modulating by a new chemical entity for new drug candidate development.

Authors acknowledge the High-End Computation Facility and Schrodinger2022/Gaussian 16 Software support from BIT Mesra.

References.

[1] Verba KA, Wang RY-R, Arakawa A, Liu Y, Shirouzu M, Yokoyama S, Agard DA (2016) Atomic structure of Hsp90-Cdc37-Cdk4 reveals that Hsp90 traps and stabilizes an unfolded kinase. Science 352 (6293):1542-1547. doi:10.1126/science.aaf5023

[2] Oláh J, Szénási T, Lehotzky A, Norris V, Ovádi J (2022) Challenges in Discovering Drugs That Target the Protein–Protein Interactions of Disordered Proteins. International Journal of Molecular Sciences 23:1550. doi: 10.3390/ijms23031550

[3] **Schrödinger Release 2022-3**:Schrödinger, LLC, New York, NY, 2021.

Ashoke Sharon (born 1975, India), after a Ph.D. in the area of Medicinal Chemistry from CSIR-CDRI, Lucknow (2004), moved to Drug Discovery Group, University of Georgia, USA, for postdoctoral research on the design and synthesis of carbocyclic nucleosides as an antiviral candidate. In 2009, he returned to India to join the Department of Chemistry, Birla Institute of Technology (BIT), Mesra, Ranchi, and is presently working as a Professor & Head Department of Chemistry. Dr. Sharon, a medicinal and structural chemist, published 90 papers (citation: 1350, h-index: 22) and 05 patents in collaboration with biologists. He continues his drug discovery effort with his research group (Drug Discovery Education & Research Group; www.dder.in) at the Department of Chemistry, BIT, Mesra, Ranchi. He has completed six antiviral Extramural Research Grants, and one is ongoing. His current research includes in silico simulation /modeling and synthesis of drug-like analogues for antiviral drug discovery.

Prof. Samit Guha

Design of Artificial Molecular Machines for Targeted Imaging and Health

Samit Guha

Department of Chemistry, Organic Chemistry Section, Jadavpur University,

Kolkata 700032, India

E-mail: *samit.guha@jadavpuruniversity.in , samitfsu@gmail.com*

Abstract:

A molecular machine is an assemblage of fragments that create quasi-mechanical movements in response to external stimuli. Chemistry plays an imperative part to elucidate the structure, mechanism, and function of complicated biological molecular machinery such as membrane fusion machinery, kinesin walker, RNA polymerase, ribosome, F1F0 ATP synthase etc. Noncovalent interactions can be used to assemble the parts of artificial molecular machines. It is important to control the molecular motion and convert it into mechanical work that may be activated by using chemical fuels such as pH, light, redox, heat, etc. I will present the design and construction of molecular shuttle, molecular elevator, molecular muscles, valve, molecular motor, molecular computer chip, medical nanorobots, artificial membrane fusion machinery, delivery systems, mitochondria targeting agents. 1-2 I will also present NIR fluorescent dual targeting rotaxanes which can be used for live cancer cell specific lysosomal tracking and multicolour cellular imaging. 3 I will demonstrate a pH sensitive tumour activated NIR rotaxane for photothermal cancer theranostics. In addition, these molecular machines can be further customized by incorporating drugs to make a wide array of novel laser responsive therapeutic and diagnostic agents.

References:

(1) (a) J. F. Stoddart, Angew. Chem. Int. Ed. 2017, 56, 11094. (b) J.-P. Sauvage, Angew. Chem. Int. Ed.

2017, 56, 11080. (c) B. L. Feringa, Angew. Chem. Int. Ed. 2017, 56, 11060.

(2) (a) R. S. Das, P. C. Saha, N. Sepay, A. Mukherjee, S. Chatterjee, S. Guha, Org. Lett. 2020, 22, 5839.

(b) A. Sardar,T. Bera, S. K. Samal, N. Dewangan,M. Kamble, S. Guha, P. K. Tarafdar*, Chem. - Eur. J.

2022, DOI: 10.1002/chem.202203034. (c) P. C. Saha, T. Bera, T. Chatterjee, J. Samanta, A. Sengupta, M.

Bhattacharyya, S. Guha, Bioconjugate Chem. 2021, 32, 833.

(3) (a) R. S. Das, A. Mukherjee, S. Kar, T. Bera, S. Das, A. Sengupta, S. Guha, Org. Lett. 2022, 24, 5907.

(b) A. Mukherjee, P. C. Saha, R. S. Das, T. Bera, S. Guha, ACS Sens. 2021, 6, 2141. (c) A. Mukherjee, P.

C. Saha, S. Kar, P. Guha, R. S. Das, T. Bera, S. Guha, ChemBioChem 2022, DOI:

10.1002/cbic.202200641.

Brief-Biodata

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Section, Jadavpur University, Kolkata. He obtained his PhD from Indian Association for the Cultivation of Science, India (2009). Postdoc Florida State University, Florida, USA (2010-2011) Alexander von Humboldt Fellow, postdoctoral researcher, University of Göttingen, Göttingen, Germany (2011-2013); University of Notre Dame, Indiana, USA (2014–2015)

Awards: DST-SERB Early Carrier Award (2018), Government of India; Innovator Award (2014) for US patent, USA; Alexander von Humboldt Fellow (2011-2013), Germany.

Current Research Interests: Rotaxanes, Supramolecular Machines, Molecular Recognition, Selective

Targeting and Imaging of Cellular Organelles, Mitochondria and Lysosome Tracking Fluorophores, Self- Assembling Peptides at the Target Site to Control Cellular Function, NIR Organic Biomarkers and Biosensors.

Prof. K. V. Radhakrishnan

Nature’s Inspiring Revelations for Future Technological Developments

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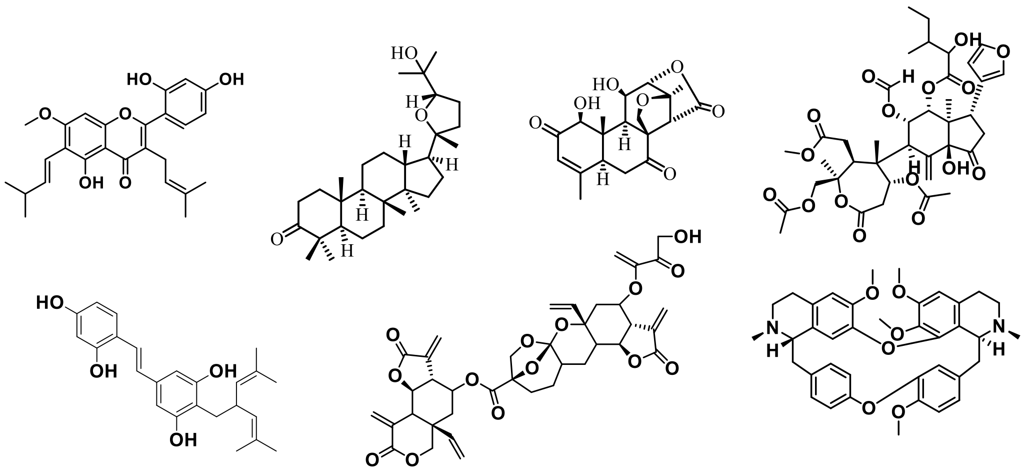
Abstract:

India’s biodiversity related to the food and health security has become the point of discussion amongst the concerned experts today. Information and knowledge on the chemistry, the availability pattern of the biochemical compounds vis-à-vis the ecology of such plant species and the nutrition value of most of the Kerala’s food and health biodiversity is woefully inadequate today. **Multi-disciplinary study** of the food and health value biodiversity available in the small holder farms or in uncultivated fields had never been a serious concern for the concerned scientists in Kerala or for that matter in the country as a whole. As a result, many of the traditionally cultivated or conserved species that have historically contributed to food, nutrition and health needs of the people (often those belonging to the poor and vulnerable sections) became neglected! It is imperative therefore for botanists, social scientists, agricultural scientists; natural product chemists, medicinal chemists, nutrition experts and biochemists to work together with the local community to produce evidence based knowledge that will help to take better decisions for the sustainable management of this dying biodiversity of India. This will lead to future technological developments in several areas especially related to food and health security.



The results of our investigation on phytochemical profiling of selected medicinal plants with its output in developing molecules against MDR strains of S. aureus and active anticancer molecules against SAS oral cancer etc will be discussed.

Dr. K. V. Radhakrishnan Professor, AcSIR, New Delhi . Senior Principal Scientist & **HOD** of Organic Chemistry CSIR-NIIST, Industrial Estate. PO. Trivandrum-19

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Education

BSc &MSc. Chemistry, Christ College, Irinjalakuda, Kerala, India (1986-1991) (University of Calicut).

Master of Human Resource Management (MHRM) from University of Kerala (2016)

Ph.D. in synthetic organic chemistry from University of Kerala (1998) under the supervision of Dr. Vijay Nair, CSIR-NIIST, Trivandrum

Ongoing PhD in Data Analytics (R&D Management) at Digital University of Kerala

Post-Doctoral Fellowships

1. Tohoku University, Sendai, Japan with Professor Yoshinori Yamamoto,
2. Molecumetics Institute, Bellevue, Seattle, WA, USA with Professor Michael Kahn
3. NPG Research Institute, Raleigh, North Carolina, USA with Professor Bert Fraser-Reid.

From 28 May 2002 onwards as Scientist at CSIR-NIIST, Trivandrum

Research interests

☐ Bio-prospecting of medicinal plants (Phytochemistry)
☐ Homogeneous and heterogeneous catalysis for industrially important molecules
☐ Synthetic carbohydrate chemistry
☐ Process innovation for APIs and crop protection chemicals
☐ Development of novel synthetic methodologies for sustainable chemistry

Awards & Fellowships

Chemical Research Society of India (CRSI) Bronze medal in Chemical Sciences for the year 2016

First Rank in Master of Human Resource Management (MHRM) from University of Kerala in 2016.

Other assignments

1. Faculty, Academy of Scientific and Innovative Research, (AcSIR), New Delhi.
2. Visiting faculty in Department of Applied Chemistry, Cochin University of Science and Technology,Kochi
3. Visiting faculty, Indian Institute of Science Education and Research (IISER, Trivandrum)
4. Visiting Faculty, Université de Reims Champagne-Ardenne (URCA),Reims, France(Indo-French collaboration)
5. Indo-Finland collaboration with University of Jyvaskyla, Finland.

Thesis Supervision and Guidance: Ph.Ds completed-31: MSc/MTech/MD (Ayu): 127 nos:
Currently supervising: **Six(6)** ongoing PhD Students(Chemistry : **2** & Biology: **4**)

Publications: Papers published/in press in peer-reviewed international/national journals **-146**
Six book chapters and **One** US patent & **Five** Indian patents filed

Dr. Prithidipa Sahoo

Designing Chemosensors for Environmental toxicants

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Abstract:

The main objective of this research work is to design and synthesis of some novel chemosensors which are highly sensitive and selective for the detection of some toxic elements in aqueous medium. The toxic elements become hazardous to the whole ecosystem through their ability of binding with vital cellular components, such as structural proteins, enzymes, and nucleic acids, and interfere with their functional activities. In consequence, a reliable, facile and reactive detection method of such hazardous species, is of great global interest towards the development of practical ‘in field’ devices. We use various types of biocompatible fluorophores such as rhodamine, coumarin, carbazole, fluorescein etc. as well as we will introduce different reactive functionalities around the binding zones depending on the reactant substrates for studying protocols of chemosensors. The selective detection of hazardous species has been a major research focus in science and technology for many decades given its myriad application in molecular diagnosis, environmental monitoring, drug discovery, and biological warfare.

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2. Reliable fuorescence technique to detect the antibiotic colistin, a possible environmental threat due to its overuse, Saurodeep Mandal, Arpan Dey Bhowmik, Alpana Mukhuty, Shampa Kundu, Khai-NghiTruong, Kari Rissanen, Ansuman Chattopadhyay & Prithidipa Sahoo*, Scientifc Reports, 2022 12, 9307

3. Involvement of a unique chemodosimeter in the selective estimation of noxious cyanide in common water hyacinth (Eichhornia crassipes): an environmental refinement, Shrabani Saha, Priyotosh Ghosh, Paritosh Mondal, Ansuman Chattopadhyay and Prithidipa Sahoo* Environ. Sci.: Processes Impacts, 2021, 23, 1308 [Selectethe d as front cover of this issue]

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Solvent- and Substrate-Induced Chiroptical Inversion in Amphiphilic, Biocompatible Glycoconjugate

Angshuman Ghosh

Abstract:

We have shown solvent- and substrate-dependent chiral inversion of a few glycoconjugate supramolecules. (Z)-F-Gluco, in which D-glucosamine has been attached chemically to Cbz-protected L-phenylalanine at the C terminus, forms a self healing hydrogel through intertwining of the nanofibers wherein the gelators undergo lamellar packing in the β-sheet secondary structures with a single chiral handedness. Dihybrid (Z)-F-gluco nanocomposite gel was prepared by in-situ formation of silver nanoparticles AgNPs in the gel; this enhances the mechanical properties of the composite gel through physical crosslinking without altering the packing pattern. In contrast, (Z)-L-gluco bearing an L-leucine moiety does not form a hydrogel but an organogel. Interestingly, the chiral handedness of the aggregates of (Z)-L-gluco can be reversed by choosing suitable solvents. In addition to self-healing behavior, (Z)-Lgluco gel revealed shape persistency. Further, (Z)-F-gluco hydrogel is benign, nontoxic, non-immunogenic, and non-allergenic in animal cells. AgNP-loaded (Z)-Fgluco hydrogel showed antibacterial activity against both Gram-positive and Gram-negative bacteria.

Zinc Acetate-Promoted Blocking of ATRA Process with Alkyl Halides Enabling Photochemical Alkylamination of Olefins

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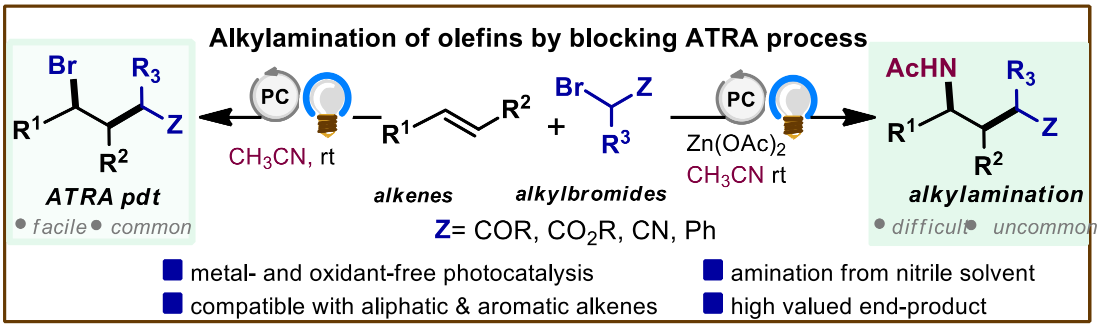
Organic photoredox-catalyzed alkylamination of olefins is performed with alkyl halides and nitrile solvent by blocking the traditional photoredox-ATRA process with $Zn(OAc)_2$. A range of carbon-centered radicals (α-alkylcarbonyl, benzyl, cyanomethyl) are effectively participating in this strategy giving rise to versatile carboamination products with high synthetic value.



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g-C3N4 Catalyzed Photo-Decarboxylative Functionalization of Benzylic C(Sp3)-H with carbonyl moiety: - An Alternative of Grignard's Reaction

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Abstract:

The Grignard reaction is an organometallic chemical reaction in which alkyl, allyl, vinyl, or aryl magnesium halides (Grignard reagent) is added to a carbonyl group in an aldehyde or ketone.1 We demonstrated a metal free heterogeneous organic semiconductor g-C3N4 catalysed2,3 and visible light-assisted benzylation of carbonyl moiety. A facile reaction results in the construction of C−C bonds4 under mild conditions in blue LED irradiation. The catalysis initiates via a radical pathway and involves a ketyl radical anion intermediate.5 The reaction shows good functional group tolerance with excellent yields. The strategy provides an easy access to these molecules with potential medicinal chemistry applications.

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Unusual and Stable Locking of Tautomeric Fluorinated Diazo Compound During Photo Switching: Solvent Assisted Photochromism

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Abstract:

Molecular switches, which enable the storage of information on a molecular level have developed a considerable interest in recent year due to its wide application in photo controllable catalysis, solar light harvesting, photo-pharmacology, optical-to-mechanical energy conversion, molecular electronic and photonic devices etc. Molecular switches are addressed by a chemical or photochemical reactions to specifically switch the physical and chemical properties between two states and *trans-cis* isomerization of azo-benzene is a representative example. Although there are many others, but azobenzene emerged as the top compound due to many inherent reasons like their easier synthetic methods, high extinction coefficients, high isomerization quantum yields, change in dipole moment upon photoisomerization, and high fatigue resistance.

Generally, azobenzene undergoes photoisomerization from *E* to *Z* *via* π- π* transitions which generally lead to a decrease in the intensity of π- π* band with blue shift and increase of intensity of *n*- π*band, while *Z* to *E* transformation proceeds *via* either photochemical or thermal way.

Recently, we observe that unprotected phenolic azobenzene showed unusual photochromism under polar solvent and instead of *trans-cis* isomerization, compound undergoes switching between *enol-azo* to *keto-hydrazo* isomerization and *vice-versa* under photochemical and thermal condition respectively. More surprisingly, when we used fluoro derivative then photo-switching process was ceased after only light irradiation and stable *keto-hydrazo* was formed. The above observation was highly dependent on the type of solvent used. Thus, when non-polar solvent like benzene was used then in both cases, a regular *trans-cis* photo-switching were observed. A mechanistic investigation was properly done to understand the above observation.

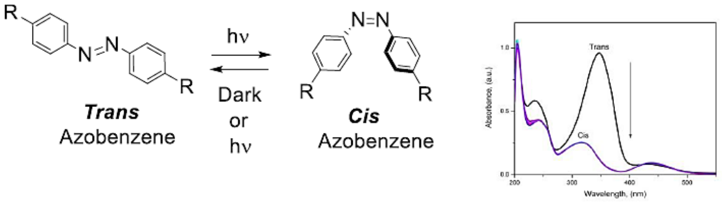

Figure 1: *trans-cis* photoisomerization and characteristic change in UV-visible spectrum.

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Aza-BODIPY Self-Assemblies with Switchable Fluorescence Activity

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Abstract:

Aza-BODIPYs has been known for decades now but only a few reports have done in regards to its targeting purpose for cancer diagnosis. In these regards, a self-assembly of aza-BODIPY-biotin bioconjugate for bioimaging has been designed and developed. The bioconjugates displayed favorable absorptions in the photobiological window and had specific turn on fluorescence characteristics with specific recognition biomarkers. *In vitro* investigations of these bioconjugates revealed fast cellular uptake, effective optical imaging, with minimal cytotoxicity in biotin receptor positive MDA-MB-231 breast cancer cells.

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Chloroform-COware Chemistry: An Emerging Technique for Palladium-Catalyzed Aminocarbonylation

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Abstract:

The carbonyl group forms an integral part of several drug molecules and materials; hence, synthesis of carbonylated compounds remains an intriguing area of research for synthetic and medicinal chemists. Handling toxic CO gas has several limitations; thus, using safe and effective techniques for in or ex situ generation of carbon monoxide from nontoxic and cheap precursors is highly desirable. Among several precursors, chloroform can prove to be a promising CO surrogate due to its cost-effectiveness and ready availability. However, the one-pot chloroform-based carbonylation reaction requires strong basic conditions for hydrolysis of chloroform that may affect functional group tolerability of substrates and scale-up reactions. These limitations can be overcome by a two-chamber reactor (COware) that can be utilized for ex situ CO generation through hydrolysis of chloroform in one chamber and facilitating safe carbonylation reactions in another chamber under mild conditions. The versatility of this "Chloroform-COware" technique is explored through palladium-catalyzed aminocarbonylation of isoquinoline and quinoline.

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Mechanochemisty-driven catalyst- and solvent-free Csp2-H functionalization of 4-hydroxycoumarins via C-3 dehydrogenative aza-coupling

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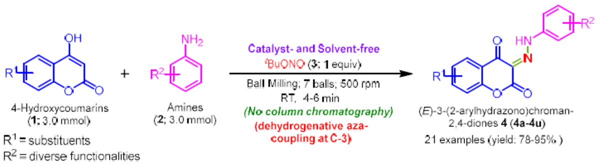
Abstract:

The generation of carbon-heteroatom bonds is fundamental for synthesizing bioactive natural products, pharmaceuticals and useful materials. Among various synthetic strategies for constructing carbon-heteroatom bonds, the desired C–H bond functionalization within diverse molecular scaffolds has already emerged as an advantageous and fascinating protocol in modern organic synthesis. The last decade has witnessed considerable advances in mechanosynthesis involving a wide array of covalent bond-forming reactions, and the application of this green tool featured a handful of advantages, including avoidance or reduced use of bulk organic solvents, shortened reaction time, enhanced yields, improved selectivity, and minimized ecological impacts. The present work deals with designing and developing a new protocol for synthesizing biologically relevant coumarin-hydrazones by a three-component reaction between 4-hydrocoumarins, primary aromatic amines and tert-butyl nitrite under ball-milling in the absence of any catalyst/additive and solvent (Scheme 1). The mechanic force implements the Csp2-H functionalization of 4-hydroxycoumarins via C-3 dehydrogenative aza-coupling with ease. The process bears a lot of advantages that include the catalyst- and solvent-free reaction conditions, the use of ball-milling as a green tool, no need for chromatographic purification, broad substrate scope and tolerance for various functional groups, high yields of products at short reaction times (no more than 6 min), clean reaction profile, and gram-scale synthetic applicability.



Scheme 1. Mechanochemistry-driven C_{sp2}–H functionalization of 4-hydroxy-coumarins

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Exploring Eosin Y as a bimodular catalyst: organophotoacid mediated Minisci-type acylation of N-heteroarenes

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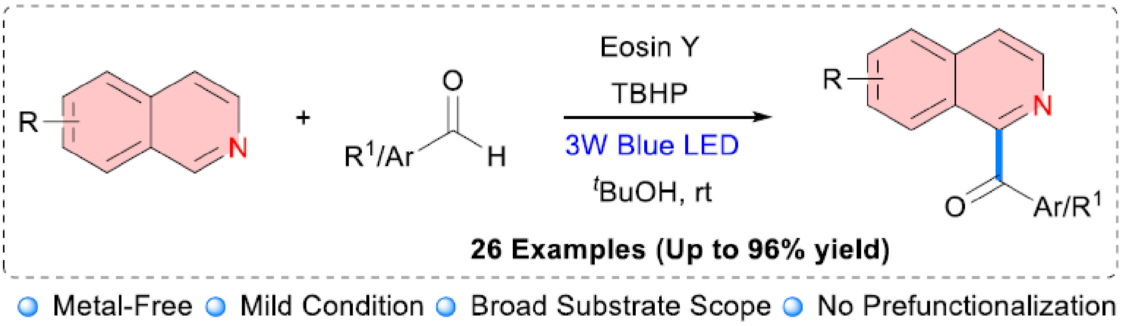
Abstract:

Here we report Eosin Y as a bimodular catalyst for Minisci-type acylation reactions. The formation of organic exciplexes between photoexcited Eosin Y and N-heteroarenes was found to be a stabilizing factor for photoacid catalysis under optimized conditions. Spectroscopic investigations such as steady state fluorescence quenching and dynamic lifetime quenching experiments were employed to better understand the role of Eosin Y as both a photoredox catalyst and a photoacid. Feedstock aldehydes were employed as acyl radical precursors for engaging in C–C bond formation reactions with a variety of nitrogen containing heterocycles.



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Design and Synthesis of Novel Photoswitchable Molecules Enabling Reversible Optical Control of Protein Labeling: A Promising New Direction in Photopharmacology

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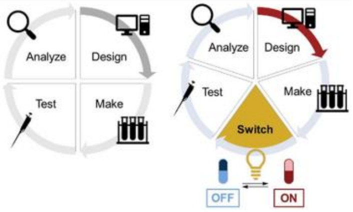
Abstract:

Proteins account for the most important molecules in living organism by functioning through interaction with numerous biomolecules. Thus, understanding the structure, distribution, trafficking and functions of protein of interests (POIs) in living cells is one of the fundamental goals of chemical biology research. Protein labeling systems that specifically label a tag-fused POI with a functional small-molecule have been proven to be versatile methods for elucidating protein functions in living cells. However, it is difficult to apply them to repetitive control of the protein functions because of their irreversibility. As the emerging technology, photopharmacology provides a uniquely powerful means to enable the optical control of biological processes in living cells with high spatiotemporal resolution.1 To overcome the limitation of irreversibility, a new chemical biology tool, incorporating the primary concept of photopharmacology, for reversible optical control of protein labeling is of utmost importance. Aiming to develop the desired photoswitchable protein labeling system, we have developed a set of novel ligands that can reversibly bound to a selective protein on the basis of photochromism.

Escherichia coli dihydrofolate reductase (eDHFR), a key enzyme in the folate metabolism, has been established as a promising tag protein.2 Recently, we have reported a photoswitchable ligand, azoMTX, that can efficiently bind with eDHFR and can switch its enzyme activity.3 However, azoMTX also binds to human DHFR (hDHFR) and inhibits the activity.4 This property would hinder the application of azoMTX as a chemical tool in human cells. Therefore, a new set of photoreversible molecules, **azoPyQ**s, capable of selective binding to eDHFR, will be presented in this conference. The newly synthesized compounds reversibly isomerize upon UV light (394 nm) and green light (560 nm) irradiation and offer high thermal stability of the active *Z*-isomers. The new compounds also show reversible optical control of eDHFR enzyme activity inhibition, while almost no activity change in case of hDHFR.5 One of the compounds in its active *Z*-isomeric form exhibits more than 21 times higher affinity to eDHFR than hDHFR, indicating the selectivity of binding to eDHFR. Thus, our newly developed eDHFR-selective photoswitchable inhibitors will be useful as a next-generation chemical biology tool in developing photoreversible protein labeling systems.



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Catalyst Switchable Divergent Synthesis of Bis(indolyl)alkanes and 3-Alkylated Indoles from Styrene Oxides

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Abstract:

A novel and effective Brønsted acid-catalysed chemo selective synthesis of bis(indolyl)alkanes and 3-alkyl indoles are reported. The selectivity of two significant indole derivatives is attained by allowing the same substrates to go through divergent reaction routes catalysed by different catalysts. Furthermore, a wide range of bis(indolyl)alkanes and 3-alkyl indoles were afforded in moderate to good yields, demonstrating good substrate universality. It was concluded from control experiments and *in-situ* IR study that in the presence of Brookhart's acid, the phenyl oxirane rearranged to phenylacetaldehyde as an intermediate. Moreover, the bisindoylation reaction occurs promptly at room temperature. This reaction was found to be scalable with good efficiency.

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Intramolecular Oxidative C−N Bond Formation under Metal-Free Conditions: One-Pot Global Functionalization of Pyrazole Ring

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Abstract:

An efficient DTBP promoted and NaI-catalysed, greener protocol for the synthesis of highly substituted pyrazoles *via* C(sp2)–H bond functionalization has been reported. This protocol is general and the reaction efficacy improves significantly with the combined use of solvents *t*-BuOH and EtOH, producing a vast variety of substituted pyrazoles in good to excellent yields. The mechanistic investigations including the radical trapping experiment indicating the *in-situ* generation of intermediate free-radical species followed by intramolecular oxidative C−N bond formation afforded the desired pyrazole moiety. The synthetic versatility of this methodology is further highlighted by preparing a diverse range of substrates including di-/tri-/and tetra-substituted pyrazoles, and applying the methodology in the practical synthesis of bioactive scaffolds.

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Transforming Non-Innocent Phenalenyl to a Potent Photoreductant: Captivating Reductive Functionalization of Aryl Halides through Visible Light-Induced Electron Transfer Processes

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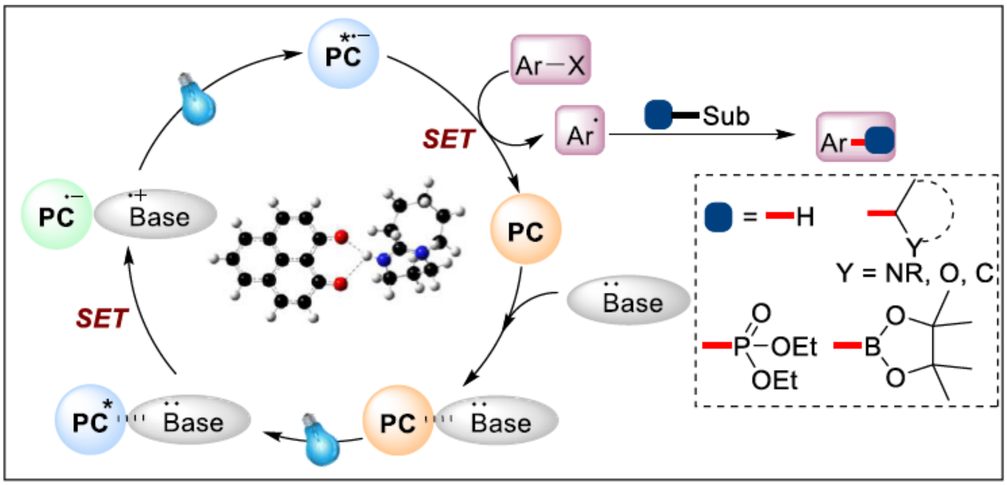
Abstract:

We have established a phenalenyl based molecular scaffold which serves as a potent photoreductant utilizing the NBMO in presence of base to form a radical anion which upon photoexcitation behaves as a stronger reductant and accomplishes the cleavage of strong C-X (X=Cl,Br,I) bonds under milder reaction conditions. Base was found to be involved in a dual role of electron and hydrogen atom donor. Further, the aryl radical formed by homolysis of C-X bonds was captured for C_{sp2}-C_{sp2} coupling with unactivated arenes. The photoreductant potency of the phenalenyl based catalytic system was further extended to C-P and C-B bond formation reactions. EPR and lifetime studies reveal the formation of a persistent radical having sufficient lifetime to take part in the reaction by photoinduced electron transfer (PET) mechanism. Different spectroscopic techniques combined with DFT calculations were utilized for characterization of active catalytic species and elucidation of plausible mechanistic pathway.



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Lewis Acid Promoted Homodimerization of Styrene Diols: An Efficient Approach toward 2-Phenylnaphthalenes

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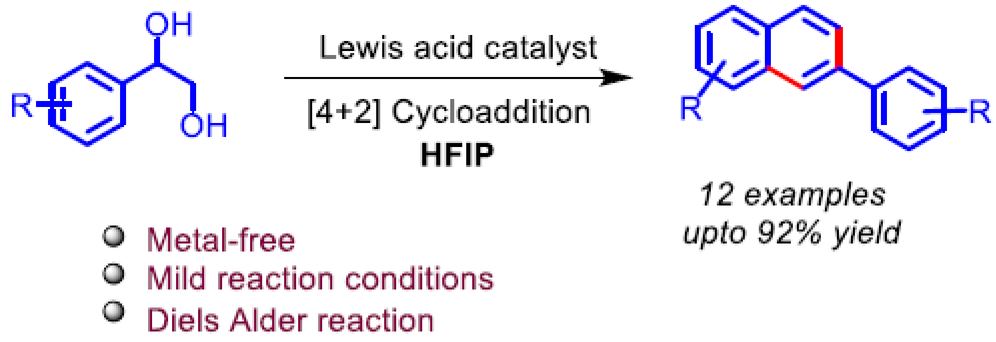
Abstract:

The privileged 2-phenylnaphthalene molecule has received significant interest due to its potent estrogen receptor (ER-b) agonistic properties. Herein, we report a straightforward, metal-free, efficient protocol for the synthesis of 2-phenylnaphthalenes from 1-phenylethane- 1,2-diols under mild conditions. In this present synthetic strategy, 1,1,1,3,3,3-hexafluoro-2- propanol (HFIP) is used as a solvent that stabilizes the reaction intermediate. The mechanism of this reaction has been studied by an *in-situ* IR experiment that revealed that the reaction proceeds through the formation of phenylacetaldehyde. The process involves an intermolecular [4+2] Diels–Alder reaction. HFIP as a solvent helps to stabilize the reaction intermediates for this cycloaddition. Moreover, this dimerization works under mild conditions with inexpensive catalysts and it provides excellent yields. Several control experiments were performed to gain mechanistic insights into the reaction.



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Catalytic Direct Cyanomethylenation of C(sp3)−H Bonds via One-Step Double C-C Bond Formation

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Abstract:

Enenitrile compounds, specifically functionalized acrylonitriles, play a central role as synthetic intermediates in organic chemistry.1 Both conventional and modern synthetic approaches for enenitrile compounds demand substrates that bear reactive sp2- or sp-hybridized carbon centers. 2 We report a unique one-pot cyanomethylenation of C(sp3)−H bonds adjacent to azoles and ketones via two consecutive C-C bond formations using DMF as the methinylating (=CH) source and TMSCN as the cyanating source under Pd/Cu bimetallic catalysis.3 Some noteworthy features include: 1. C(sp3)–H bonds next to benzoxazoles and benzothiazoles are operational, 2. Broad substrate scope – >30 examples; achieved extraordinary levels of functional group tolerance and regiospecificity towards □-C–H bond; 3. A Cu-catalyst promotes the activation of C(sp3)-H bond of DMF producing "CNCH=" equivalent that undergoes a Pd-catalysed C-C bond formation with the benzazole counterpart; 4. Interconversion of cyanomethylenated products led to numerous practically useful intermediates that are otherwise challenging to access.

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Dual Metallation in a Two-Dimensional Covalent Organic Framework for Photocatalytic C–N Cross-Coupling Reactions

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Abstract:

Covalent organic frameworks (COFs) are a promising toolbox in the field of heterogeneous catalysis.[1] Herein, we report a dual metallation (iridium and nickel) strategy in a single 2D-COF TpBpy to perform a variety of C−N cross-coupling reactions.[2] Moving from the traditional approach[3], we focus on the COF-backbone as a host for metal-catalyzed photosensitive C−N coupling reactions. The controlled metallation and recyclability without deactivation of both catalytic centers are unique with respect to previously reported coupling strategies. We performed various photoluminescence and electrochemical studies with Hammett correlations to understand the mechanism. The developed protocol enables selective and reproducible coupling of a diverse range of amines (aryl, heteroaryl, alkyl), carbamide, and sulfonamide with electron-rich, -neutral, and -poor (hetero)aryl iodides. Keeping this strategy in perspective, we explored the activity to produce non-steroidal anti-inflammatory drug Fulfenamic acid, strong pharmacophore N,5-diphenyloxazol-2-amine, Food and Drug Administration (FDA) approved drugs Flibenserin, Tripelennamine and did late-stage diversification of the derivatives of ibuprofen, naproxen, gemfibrozil, helional, glycine, and ε-aminocaproic acid.

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Silver(I)-Salt Catalyzed Selective Hydroboration of Isocyanates, Pyridines, and Quinolines

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Abstract:

Organoboranes are one of the versatile precursors in synthetic chemistry as they are widely employed in the synthesis of pharmaceuticals, agrochemicals, polyesters, dyes, natural products etc.1 Among various potent functionalities, isocyanate is one of the least explored heterocumulenes for hydroboration and only three catalyst systems are known.2-4 These systems suffer from some drawbacks such as low functional group tolerance, higher catalyst loading, limited substrate scope, and require specially designed ligands. Keeping all the above-mentioned disadvantages of the previous reports, herein, we report a simple silver salt catalysed ligand-free selective mono- and deoxygenative hydroboration of isocyanates under mild conditions. Further, we explored the suitability of our protocol in pyridine hydroboration which regioselectively produces 1,4-hydroborated pyridines, playing an essential role in biological systems and as a reducing agent in organocatalysis. Additionally, the present protocol also works well for the double reduction of quinolines which upon hydrolysis produces 1,2,3,4-tetrahydro quinolines, integral components of numerous natural alkaloids, bioactive molecules, pharmaceuticals (Figure 1)

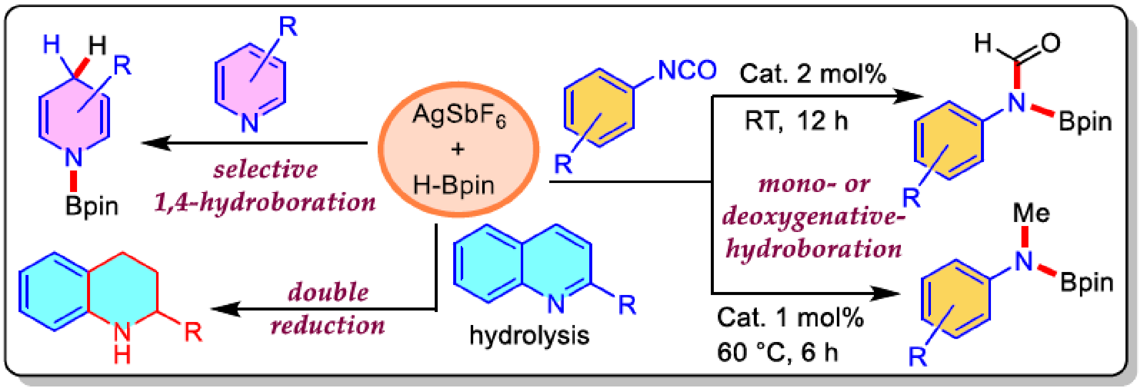

Figure 1: Schematic presentation of the present work

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Design and synthesis of Phenothiazine based functional organic push-pull molecules and their applications

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Abstract:

In recent years, multi-functional fluorescent organic compounds have become important in the fields of optical sensors, mechano-sensors, data storage, security papers, etc. Solvent polarity has a significant impact on the charge transfer phenomenon and, as a result, affects the optical properties of the D-π-A molecules. We have designed and synthesized multi-stimuli responsive fluorescent organic materials by phase transfer Heck coupling reaction.1 Intramolecular charge transfer from donor to acceptor in a highly polar medium results in the formation of the relaxed perpendicular state by twisting (TICT),2 which is responsible for TICT-induced moisture detection in three organic solvents.3 Considering the harmful effects of volatile small organic molecules such as trifluoroacetic acid and amines, their highly sensitive detection becomes very important. These compounds are employed as a turn-on fluorogenic sensor for the selective detection of triethylamine and *n*-dibutylamine vapours. They also exhibit reversible acidochromism4 in both solution and solid-state.

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Chemosynthetic Livers: Predict, Prepare, and Prove the Structure, Activity, and Toxicity of Drug Metabolites – New Results

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Abstract:

We report advances in proprietary *in-vitro* green chemistry-based technology, mimicking *in-vivo* metabolism of several chemical entities used in pharmaceuticals, cosmetics, and agrochemicals. Our catalysts enable prediction of metabolism patterns with soft-spot analysis and the methodology introduces new paradigms for drug discovery and drug-drug interactions for clinical diagnostics. Metabolites are implicated in adverse drug reactions and are subject to intense scrutiny in drug R&D. Present-day processes involving animal studies are expensive, labor-intensive, and chemically inconclusive. Our catalysts (azamacrocyclic) are sterically protected and electronically activated providing speed, stability, and scalability. We predict structures of metabolites, prepare them on a large scale by oxidation, and elucidate chemical structures. Comprehensive safety evaluation enables researchers to conduct more complete in vitro metabolism studies, confirm structure and generate quantitative measures of toxicity. We define an animal-free platform that identifies a more complete set of safety-relevant drug metabolites to accelerate the pace of drug discovery and metabolism.

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Carbon-carbon and Carbon-heteroatom Bond Formation Reactions under Green Conditions

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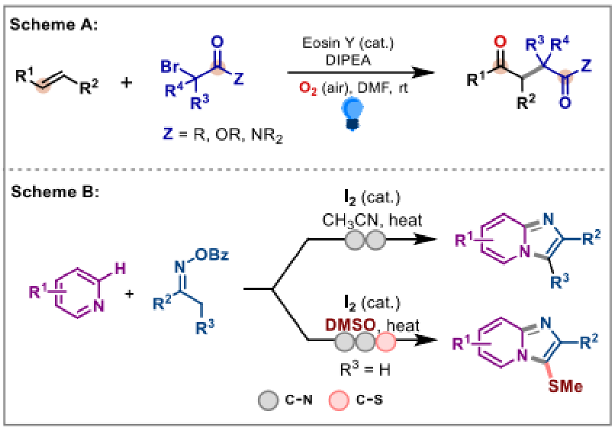
Abstract:

1,4-Ketocarbonyl compounds have proven themselves a very interesting and versatile building block to access various important carbocyclic as well as heterocyclic compounds.[1] We have developed a metal free protocol to access 1,4-ketocarboyl compound through oxidative radical coupling of styrenes with diverse bromocarbonyls under photoredox catalysis [Scheme A].[2] The method is mild, operationally simple, chemo-selective and exhibits broad substrate scope with excellent functional group compatibility. In addition to that, molecular iodine catalysed synthesis of imidazo-heterocyclic and its regioselective C-3 Sulfenylated products were executed from simple pyridines with oxime-esters through formation of iminyl radical [Scheme B].[3]



Keywords: Metal free, Photoredox catalysis, 1, 4 ketocarbonyls, Iodine, Imidazo-heterocycles.

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Electrochemical regioselective C(*sp2*)-H chalcogenation of substituted 2-amino-1,4-naphthaquinones

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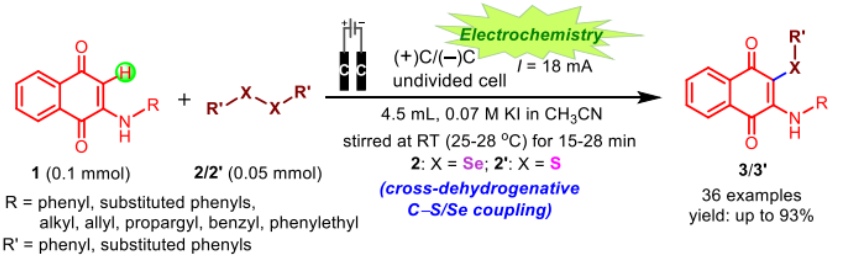
Abstract:

Oraganochalcogenides occupy a prominent position among bioactive natural and synthetic analogues with multifaceted applications. Hence, a good deal of synthetic endeavours for constructing C-S/Se/Te has been reported in the recent past. Our literature survey showed that 2,3-difunctionalized 1,4-naphthoquinones, particularly the 2,3-thioaminated versions, have already emerged as a promising class of organosulfur compounds having potent biological and pharmaceutical activities and finding applications as functional materials and useful synthones in organic synthesis. We also found that synthetic methods for this important building block are still very limited. Hence, we felt it pertinent to develop a general methodology for the chalcogenaton of this important bioactive organic scaffold as part of our ongoing endeavours in synthesizing functionalized diverse organic motifs following green chemistry concepts. Recently, we have successfully unearthed an electrochemical strategy as an alternative method for accessing the 2,3-thioaminated version of 1,4-naphthoquinones and a new series of 2,3-selenoaminated analogues. The process involves regioselective C(*sp2*)-H selenylation and sulfenylation of substituted 2- amino-1,4-naphthaquinones **(1)** via oxidative cross-coupling between the substrates **1** and diversely substituted diselenides **(2)**/disulfides **(2′)** in an electrochemical cell using low-cost and readily available KI as the electrolyte as well as redox-mediator in acetonitrile at ambient temperature **(Scheme 1).** The application of electrochemical strategy has recently emerged as a hot research topic in synthetic methodology, and this technique has already offered an effective alternative to conventional methods in oxidative C-H functionalization reactions.



Scheme 1. Electrosynthesis of 3-selenylated/sulfenylated derivatives of 2-amino-1,4-naphthaquinones

Related Literature:

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2 Mandal, M.; Brahmachari *G. J. Org. Chem.* **2022**, 87, 4777-4787.
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4 Brahmachari, G.; Karmakar, I.; Karmakar, *P. Green Chem.* **2021**, 23, 4762-4770.

Decarboxylative C-4 phosphorylation of coumarin-3-carboxylic acids under ball milling

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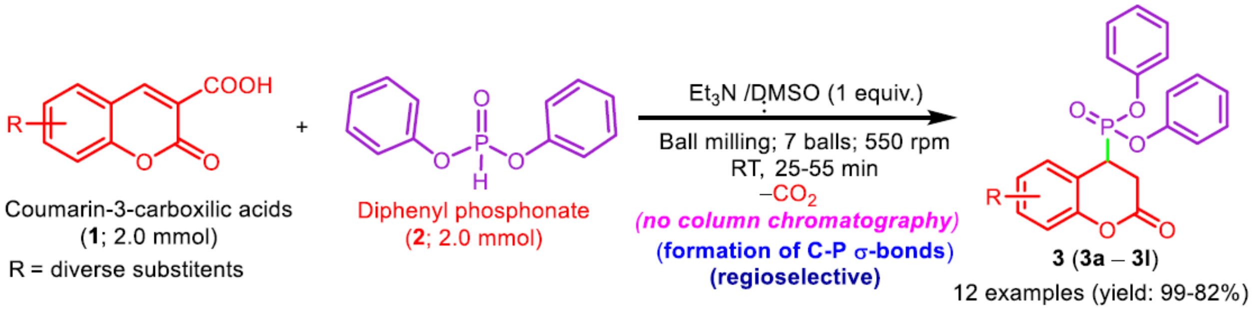
Abstract:

Chemical and pharmaceutical profiles of coumarins, either synthetic or natural, are well-established in the literature. This *O*-heterocyclic motif constitutes the basic structural frameworks of many bioactive molecules with pharmacological, food, perfumes and cosmetics, and agrochemical applications. 3,4-Dihydrocoumarin, a sub-class of this group of *O*-heterocycles, is also ubiquitously found both in natural and synthetic analogues possessing a wide range of biological profiles. Similarly, phosphorus-functionalized organic compounds always invoke immense interest in diverse groups of researchers for their useful applications in industrial, agricultural, materials, and medicinal chemistry. The imposition of a phosphoryl group on varying classes of organic skeletons thus remains a valid and active exercise in chemical research. Hence, a good deal of research has recently been reviewed on tethering a coumarin system and a phosphoryl group to open a route to a new class of organophosphorus compounds.

Recently, the ball mill application as a green tool has received much attention. The present work deals with a ball-milling-assisted straightforward and practical method for synthesizing a new series of substituted diphenyl (2-oxochroman-4-yl)phosphonates, through decarboxylative C- 4 phosphorylation of coumarin-3-carboxylic acids in the presence of triethylamine as an *N*-base additive (**Scheme 1**). The salient features of this protocol are faster reaction time, good to excellent yields, high chemo- and regioselectivity, high atom economy, operational simplicity without the use of column-chromatographic purification, eco-friendliness, and large-scale synthetic applicability.



Scheme 1. Ball-Mill-Driven decarboxylative C-4 phosphorylation of coumarin derivatives

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Brookhart's Acid-Catalyzed Switchable Regioselective *N*-Alkylation of Arylamines/Heterocyclic Amines with Cyclopropylcarbinols by Temperature Regulation

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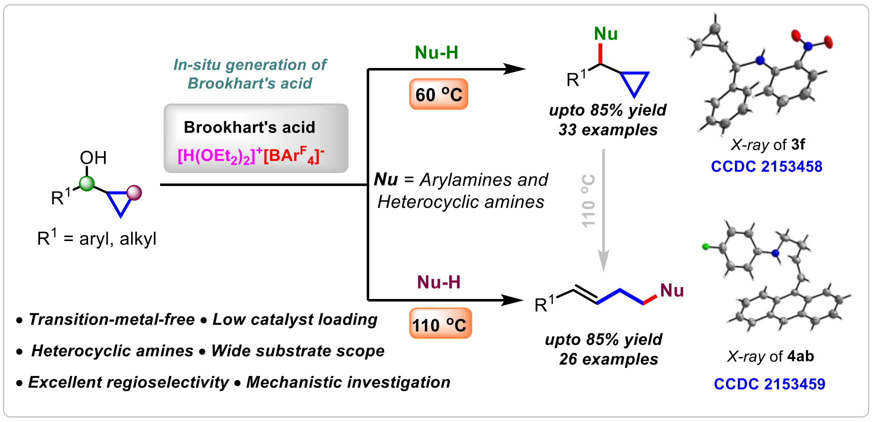
Abstract:

An unprecedented, Brookhart's acid catalyzed temperature switchable regioselective divergent approach for *N*-alkylation of arylamines and heterocyclic amines by utilising cyclopropylcarbinols is presented herein. The reaction offers *N*-alkylated cyclopropyl derivatives and homoallyl amines by employing 2.5 mol% catalyst loading at different temperatures in excellent regioselectivity and yields. This method has shown to be relevant with a wide range of cyclopropylcarbinols, including aliphatic ones. Several control experiments and spectroscopic studies have been performed to gain insight into the reaction mechanism. Further, the synthetic utility of the protocol has also been described.



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Regioselective cyclopropyl ring cleavage of tricyclo[3.3.0.02,8]octan-2-ones in BMImCl: An efficient synthesis of functionalized bicyclo[3.2.1]octanone systems

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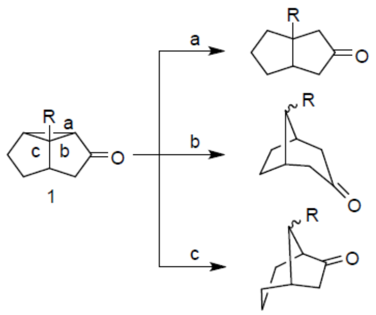
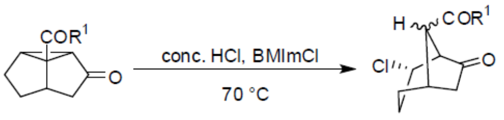
Abstract:

The regioselective cleavage of the cyclopropyl ring in tricyclo[3.3.0.02,8]octan-2-one systems provide an easy access to various cyclopentanoid natural products and their derivatives. Although in such systems, three modes of the cyclopropyl ring opening is possible (Scheme 1), the regioselectivity of the cyclopropane bond cleavage is governed by geometrical factors and the bond that is cleaved is the one that has maximum overlap with the carbonyl p-orbital. Consequently, most studies on the cyclopropane ring cleavage of such tricyclo[3.3.0.02,8]octan-2- one systems have reported the cleavage of the peripheral 'a' bond due to the aforementioned stereoelectronic reasons. The exclusive and regioselective cleavage of the cyclopropyl C1-C8 bond in tricyclo[3.3.0.02,8]octan-2-ones bearing an additional carbonyl at C1 has been carried out in BMImCl under acidic conditions to yield various bicyclo[3.2.1]octanones with amenable functional groups in both rings. Comparison of reaction in BMImCl with other conventional organic solvents clearly demonstrates the advantages of the former as the medium of choice for the regioselective cyclopropyl ring cleavage reaction.





Reference:

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Structural elucidation of phenoxybenzaldehyde derivatives from laboratory powder X-ray diffraction: A combined experimental and theoretical quantum mechanical study

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Abstract:

Crystal structure of two new phenoxybenzaldehyde derivatives, 4-(4-bromophenoxy)benzaldehyde (**1**) and 4-(4-nitrophenoxy)benzaldehyde (**2**), have been determined from laboratory X-ray powder diffraction data. The synergies of intermolecular C–H···O hydrogen bond, π ··· π, anion···π and lone-pair(l.p)··· π interactions assemble the molecules into supramolecular frameworks. The quantum chemical calculation has been performed to analyse and characterize weak noncovalent interactions in the molecules. Analysis of Hirshfeld surfaces of the compounds showed that the crystal structures are primarily characterized by H···H, H···C and H···O contacts. Bader's theory of 'atoms-in-molecules' (AIM) is applied to describe the noncovalent interactions for (**1**) and (**2**). The supramolecular frameworks are further characterized by theoretical 'Noncovalent Interaction' (NCI) plot index.

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Total Synthesis of Oridamycin A via a Late-Stage C-N Bond Formation

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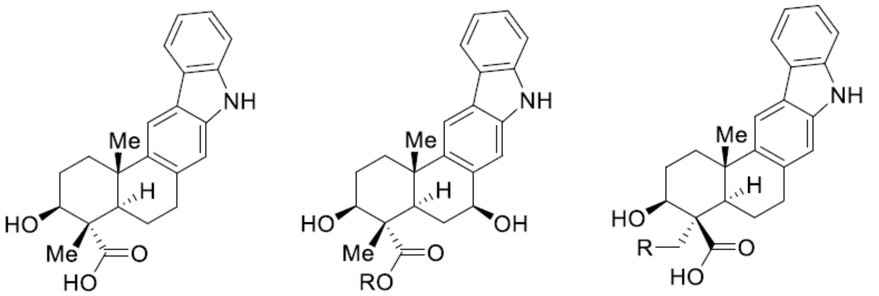
Abstract:

The xiamycins and oridamycins are secondary metabolites (Figure 1), which were first isolated from a range of Streptomyces species in 2010. These molecules represent the first examples of indolosesquiterpenoids from bacterial sources, and new members remain to be discovered. The emerging biological activity of these indolosesquiterpenoids has sparked interest in employing them as a starting point for the development of pharmaceuticals and agrochemicals. For example, xiamycin A (1a) displays antibiotic and anti-HIV activity, whereas its C-16 epimer, oridamycin A (2a), exhibits modest activity against the water mold Saprolegnia parasitica. Structurally, these pentacyclic molecules possess a carbazole nucleus fused to a trans-decalin ring system containing four contiguous stereocenters, including two quaternary centers. The major difference between the family members manifests at the C16 quaternary center; oridamycin A (2a) and oridamycin B (2b) each bear an axial carboxylic acid and an equatorial methyl/ hydroxymethyl, while xiamycin A (1a), xiamycin C (1b) contain an axially disposed methyl and an equatorial acid (Figure 1)



xiamycin A (**1a**)

R = H, xiamycin C (**1b**)
R = Me, xiamycin D (**1c**)

R = H, oridamycin A (**2a**)
R = OH, oridamycin B (**2b**)

Scheme: Naturally occurring indolosesquiterpene alkaloids (**1-2**).

In this synthesis Corey's asymmetric polyene cyclization of a triene precourser, catalyzed by $SbCl_5$ -(R)-o,o'-dichloro BINOL (1:1), which afforded carbotricyclic core bearing a trans-decalin motif and three contiguous stereogenic centers in 92% ee in 84% yield. Via a diastereoselective methylation we could install the stereochemistry at C-16 carbon atom. In the late stage a transition-metal-free direct electrolytic C-H amination involving an electrochemically generated nitrenium ion intermediate has been used for the synthesis of carbazole unit.

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Total Syntheses of Indolosesquiterpene Alkaloids, Xiamycins A & Xiamycin A methylester

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Abstract:

A novel pentacyclic indolosesquiterpene alkaloids, growing class of architecturally complex secondary metabolites were first isolated from a range of *Streptomyces* species in 2010, exhibit important biological activities such as antimicrobial, antiviral, antitumor, immunomodulatory, and enzyme inhibitory activities are displayed by this family, which is commonly referred to as the xiamycin family of alkaloids.1 More importantly recent study reveals that xiamycin A and it's methyl ester are potentially active against SARS-CoV-2.2 These indole alkaloids, i.e. xiamycin A and its methyl ester, were isolated by Hertweck et. al. from *Streptomyces* sp. GT2002/15033a and HKI05953b which are endophytes from the mangrove plant *Bruguiera gymnorrhiza*3a and *Kandelia candel*,3b respectively. Also these alkaloids are reported to display anti-HIV and antibiotic activities.3a

Structurally, these alkaloids include a pentacyclic framework with four contiguous stereogenic centers at the *trans*-decalin scaffold that is attached with a carbazole unit. On the basis of their structural similarity to naturally occurring diterpenoid, such as 4-*epi*-triptobenzene L & Antiochic acid, we envisioned a unified approach towards the xiamycins. To synthesize Antiochic acid, here we have used Sharpless asymmetric epoxidation4 approach followed by Lewis acid assisted epoxy-ene cyclisation. Finally, by late stage beckmann rearrangement and Buchwald' oxidative C-N bond formation5 we completed the total synthesis of xiamycin A & its methylester.

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Total Syntheses of Naturally Occurring Antiviral Indolosesquiterpene Alkaloids, Xiamycins C-F via Csp^3 -H Functionalization

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Abstract

Indolosesquiterpene alkaloids (2a-d; Figure 1) are a growing class of architecturally complex secondary metabolites that were first isolated from a range of Streptomyces species in 2010.[1] A number of important biological activities such as antimicrobial, antiviral, antitumor, immunomodulatory, and enzyme inhibitory activities are displayed by xiamycin family of alkaloids.[2] In 2010, xiamycin A (1a) and its methyl ester, displaying anti-HIV and antibiotic activities, were isolated by Hertweck et. al. from Streptomyces sp. GT2002/15032a and HKI0595,2 endophytes from the mangrove plant Bruguiera gymnorrhiza[2] and Kandelia candel,[2] respectively. Later, 1a was isolated by Zhang et. al.[3] In 2016, Kim et al.[4] reported the isolation of structurally related xiamycins C (2a), D (2b), E (2c) and F (2d) from a Streptomyces sp. (#HK18) culture inhabiting the topsoil in a Korean solar saltern. Structurally, these alkaloids are composed of an architecturally intriguing pentacyclic framework with four contiguous stereogenic centers at the periphery of a trans-decalin scaffold embedded with carbazole unit.

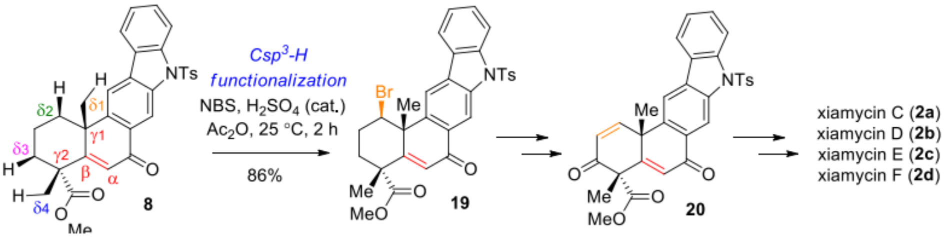

Figure 1: Naturally occurring Indolosesquiterpenoids and our approach

we have accomplished total syntheses of naturally occurring antiviral indolosesquiterpene alkaloids, xiamycins C (2a), D (2b), E (2c), and F (2d) via a late-stage oxidative δ-Csp^3 -H functionalization of pentacyclic enone 8. The synthesis of pentacyclic functionalized core of indolosesquiterpene alkaloids takes the advantage of ipso-nitration of naturally occurring abietane diterpenoids followed by a Suzuki-Miyaura reaction and a Cadogan's ring closure.[5]

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Unified Approach to the Enantioenriched Cyclotryptamine Alkaloids by Means of Thio-Urea Catalyzed Sequential Michael Reactions of Bis-Oxindoles onto Nitroethylene

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Abstract:

Hexahydropyrroloindole alkaloids comprise a large family of natural products with attractive biological activities.1 Among them, dimeric and oligomeric hexahydropyrroloindole alkaloids bearing vicinal quaternary stereogenic carbon centers at a labile and sterically hindered vicinal quaternary stereogenic carbon centers along with the structural rearrangement through a common intermediate (**3**) (Figure 1) have attracted significant interest as synthetic targets.2-3Therefore, because of their important bioactivities in addition to intriguing architecture (four contiguous stereogenic centers, see **1a-b** and **2**) there is considerable synthetic interest from the synthetic community. This resulted a number of elegant approaches including catalytic asymmetric processes.4

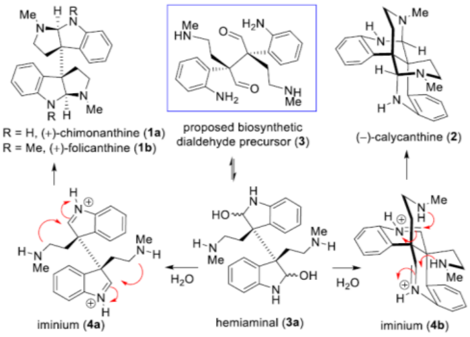

Figure 1. Dimeric cyclotryptamine alkaloids (**1-2**) and hypothetical biogenetic precursors.

We have recently developed an enantioenriched organocatalyzed double Michael addition reaction onto nitroethylene which will directly address the hexahydropyrrolo[2,3-*b*]indole scaffolds in spite of functionalization towards the amine counterpart as described in our previous report.5 Utilizing this approach, we have completed the total synthesis of both enantiomers of chimonanthine (**1a**), folicanthine (**1b**) and calycanthine (**2**).

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Asymmetric Syntheses of Bis(cyclotryptamine) Alkaloids via Thio-Urea Catalyzed Sequential Michael Addition

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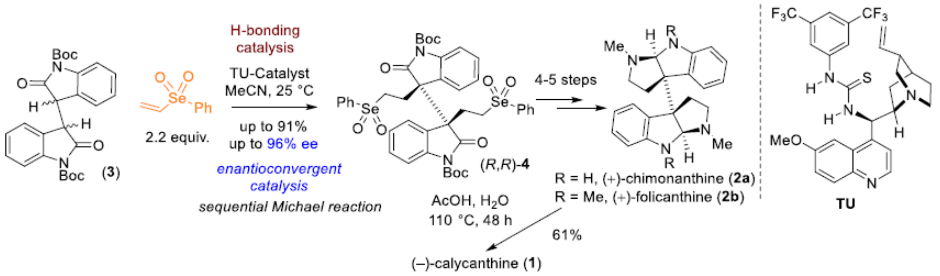
Abstract:

Bis(cyclotryptamine) alkaloids comprise a large family of secondary metabolites that are biosynthetically derived from oxidative cyclization of L-tryptophan.1 The complex bridged bicyclic structure of this family, i.e. (+)-calycanthine **1**, was first isolated *Calycanthaceae* alkaloid way back in 1888.2 However, after more than seven decades the correct structure of **1** was established by Woodward3a and Hamor,3b independently. Although other structural isomers of bis(cyclotryptamine) alkaloids, such as **2a** and **2b** have been isolated during 1960-2002.Structurally, bis(cyclotryptamine) alkaloids are characterized by the presence of vicinal quaternary all-carbon stereocenters4 at C-3a and C- 3a′ (sp3 −sp3) with six interlocked rings. A number of impressive catalytic enantioselective approaches have been reported by various research groups, including our group till date.



Scheme: Asymmetric Total syntheses of (+)-chimonanthine (**2a**), (+)-folicanthine (**2b**), and (-)-calycanthine (**1**).

Here, we have developed a thio-urea catalyzed one-pot sequential Michael addition of bis-oxindole onto selenone to access enantioenriched dimeric 2-oxindoles with vicinal quaternary stereogenic centers at the pseudobenzylic position.5 Our approach features a catalytic enantioselective synthesis of dimeric 2-oxindoles bearing vicinal quaternary stereocenters with an overwhelming control of the absolute and relative stereochemistry. This strategy has been successfully applied for the total syntheses of either enantiomer of chimonanthine, folicanthine, and calycanthine.

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"Generation & Utilization of Organic Radicals by Photocatalytic SET Process."

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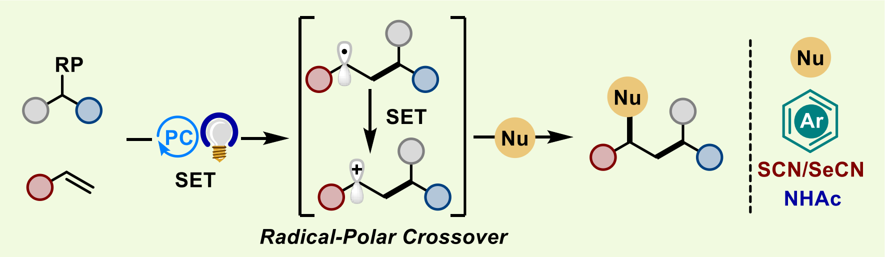

Abstract:

Photoredox-catalyzed olefin functionalization is performed with different redox-active aryl/alkyl radical precursors. First, aryl/alkyl thio(seleno)cyanation of olefin is performed using external thio(seleno)cyanation sources. Then, alkylamination of olefin is performed using nitrile solvent as aminating agent by blocking the traditional ATRA process with $Zn(OAc)_2$. Finally, carboarylation of olefin is carried out with a series of electron-rich (hetero)arenes under mild conditions.

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Organophotoredox catalysed cross dehydrogenative sulfonamidation of indoles and heterocycles

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Abstract:

Nitrogen containing heteroaryl cores are privileged structural motif found in many therapeutic drugs.1,2 Herein we reported, visible light mediated Eosin-Y catalyzed regioselective syntheses of 2-sulfonamidoindoles and 2-sulfonamido heteroarenes via oxidative cross dehydrogenative coupling (CDC) of indoles & various heteroarenes with sulfonamides. The mechanistic investigations based on control reactions, such as cyclic voltammetry and fluorescence quenching revealed that the regioselective addition of sulfonamides at the C2 position of the heterocycles takes place via the formation of nitrogen centred radical (NCR). The methodology is operationally simple, straight forward that allows the synthesis of a wide range of 2-amidated indoles along with other heterocyclic compounds.

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Total synthesis of the trisaccharide repeating unit of *Stenotrophomonas maltophilia* O6 antigen

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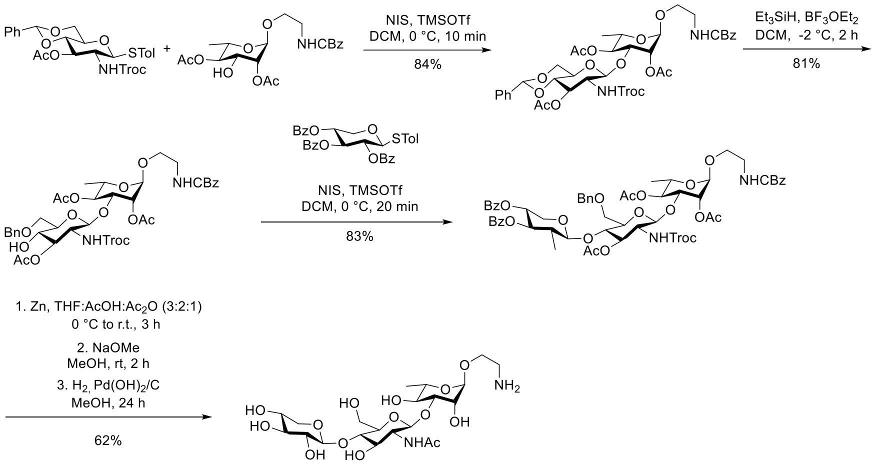
Abstract:

Research on synthetic conjugate vaccines is crucial to the prevention and incidence of diseases brought on by Gram-negative bacteria. It is essential to have access to the pure and uniform oligosaccharide fragments of the bacterial cell surface polysaccharides for the creation of such vaccines. Formerly known as *Xanthomonas maltophilia*, *Stenotrophomonas maltophilia* is an opportunistic Gram-negative rod-shaped bacillus. In immune-compromised patients, the pathogen causes nosocomial infections. Additionally, the pathogen has been reported to affect the human bloodstream, respiratory system, skin, soft tissues, biliary tract, and urinary tract. Here, we present the stepwise and one-pot synthesis of the trisaccharide repeating unit appended with 2-aminoethyl linker.



Stenotrophomonas maltophilia O6

References:

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Total syntheses of (+)- and (−)-Crinane via Palladium Catalyzed Deacylative Allylation

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Abstract:

The *cis*-3a-aryloctahydroindole alkaloids possessing an all-carbon quaternary stereo-centre constitute the core structure of many alkaloids with impressive diversity of biological activity.1 Their biological potential is significantly manifested by their anti-viral, anti-tumour, anti-cholinergic and anti-HIV properties.2 These activities together with their intriguing structures have brought a major impetus for synthetic exploration in this direction from organic chemists across the globe.3,4 The deacylative allylations (DaA) using unfunctionalized allyl alcohol is an attractive strategy for allylation of α−position of a carbonyl group. We thought of exploring this methodology for concise total synthesis of *Amaryllidaceae* alkaloids.

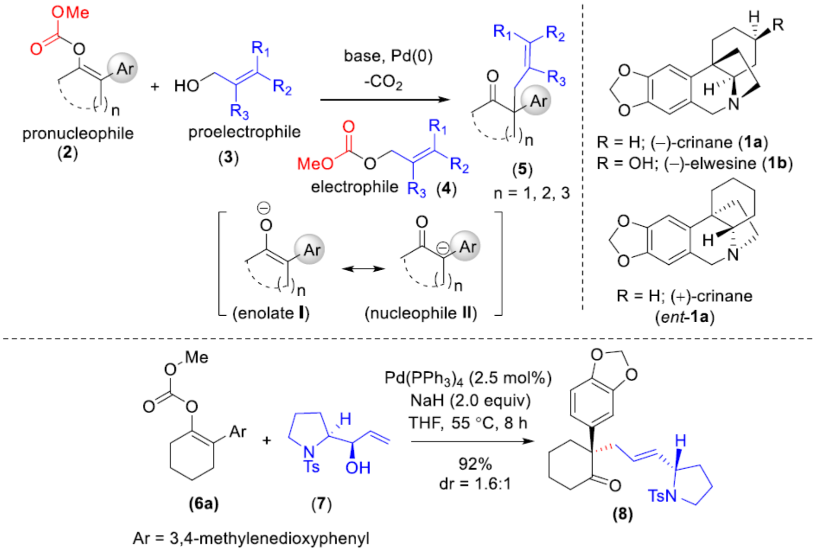

Figure: The rationale of deacylative allylations (DaA) of enolcarbonate

In this synthesis,5 we explored allylation with various substituted and unsubstituted allyl alcohols (**3**) with □-aryl (having groups both electron donating as well as electron withdrawing) substituted cyclohexanone enol carbonates (**2**) employing a Pd(0) catalyzed deacylative allylation. Further the methodology was successfully tested for deacylative benzylations. We have achieved a good to moderate enantioselectivity with good yield in most of the cases. Further the intermediate (**8**) was explored towards the syntheses of (+)- crinane (***ent*-1a**) and (−)-crinane (**1a**) following some synthetic manipulations.

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Synthesis of sugar based chiral organocatalysts and their applications in asymmetric organocatalysis

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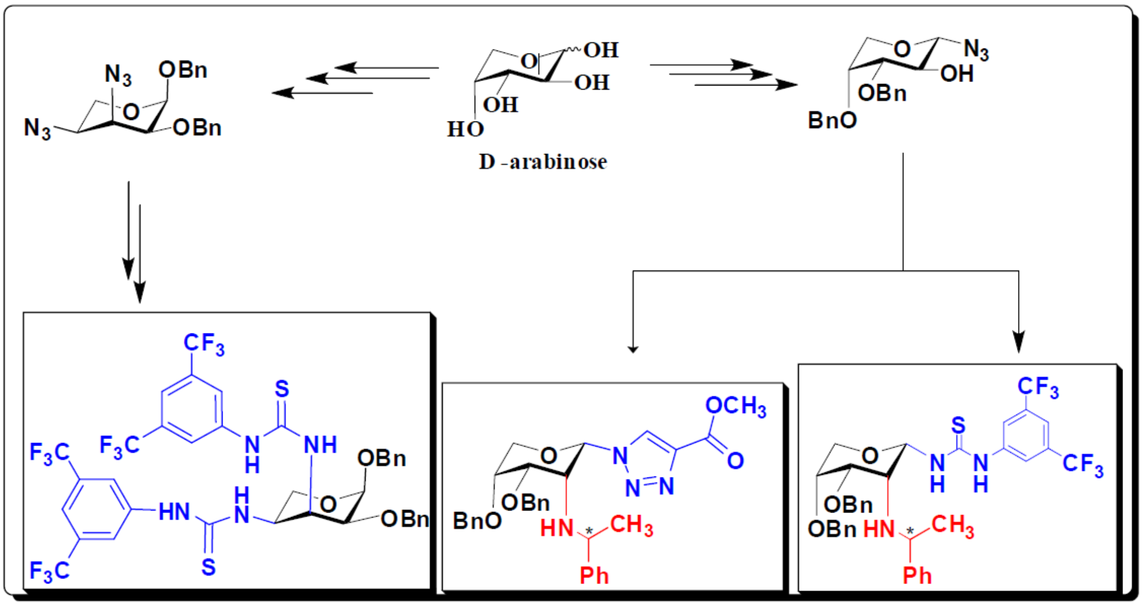
Abstract:

Chiral organocatalysts are very important tools in asymmetric synthesis. In this context, sugar moieties have been previously used as chiral organocatalysts for asymmetric induction. We have synthesised a carbohydrate based chiral *bis*-thiourea catalyst bearing thiourea moieties at C-3 and C-4 position of the sugar. We have also synthesized a sugar thiourea derivative with a vicinal chiral amine group that can function as a bifunctional chiral organocatalyst. Herein, we will report the syntheses of the target organocatalysts and their applications towards asymmetric Henry reaction.



Stereoselective synthesis of glycosyl azides from anomeric hydroxides via protecting group manipulations

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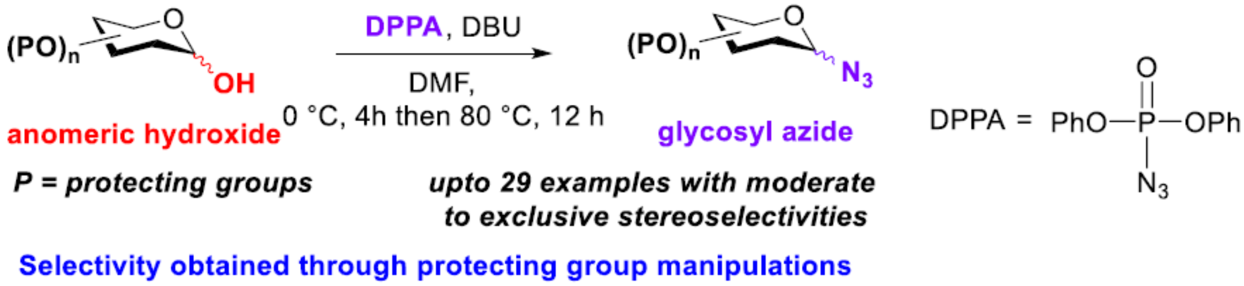
Abstract:

Glycosyl azides act as the precursors for the synthesis of *N*-glycosides, triazolyl glycosides and glycosyl ureas in carbohydrate synthesis field. Herein, we report the use of commercially available diphenylphosphoryl azide for the synthesis of glycosyl azides from anomeric hydroxides in a one-step direct method. Further, we have explored and will report the effect of different protecting groups on the stereoselectivity of the azide formation. We achieved moderate to exclusive stereoselectivities of α-/β-glycosyl azides of different hexose sugars, including β-2-deoxy-2-aminoglucosides or β-2-deoxy-2-azidoglucosides.



Aza-BODIPY Self-Assemblies with Switchable Fluorescence Activity

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Abstract:

Aza-BODIPYs has been known for decades now but only a few reports have done in regards to its targeting purpose for cancer diagnosis. In these regards, a self-assembly of aza-BODIPY-biotin bioconjugate for bioimaging has been designed and developed. The bioconjugates displayed favorable absorptions in the photobiological window and had specific turn on fluorescence characteristics with specific recognition biomarkers. *In vitro* investigations of these bioconjugates revealed fast cellular uptake, effective optical imaging, with minimal cytotoxicity in biotin receptor positive MDA-MB-231 breast cancer cells.

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Silyl Cation-Initiated, Brønsted Acid-Catalyzed Strategy towards Unsymmetrical 3, 3- disubstituted 2-Oxindoles and Azonazine Cores

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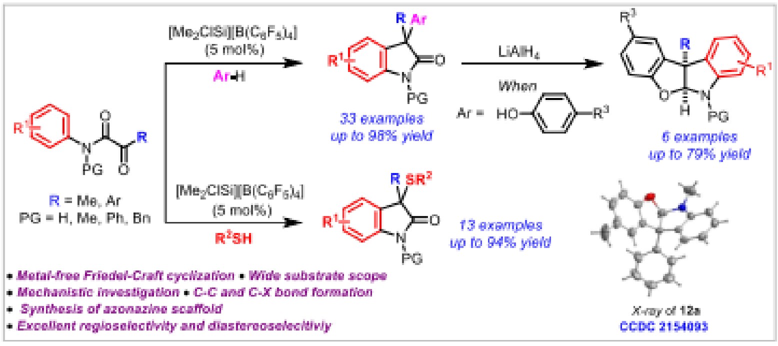
Abstract:

Herein, a mild, metal-free, robust approach for synthesizing valuable and sterically demanding unsymmetrical 3,3- disubstituted 2-oxindoles via reductive cyclization of α-ketoamides is reported. This operationally simple protocol is initiated by silyl cation and further catalyzed by Brønsted acid. We have utilized a wide range of arenes, amines, and thiols as coupling partners with various α-ketoamides. The products were afforded excellent regioselectivity and good functional group tolerance. This procedure provides easy access to the scaffolds of azonazine and its derivatives with excellent syn-diastereoselectivity bearing all-carbon quaternary stereocenters.



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Prof. Swadhin K Mandal

Small Molecules in Electron Transfer Catalysis

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Today's major concerns on the industrially used catalytic systems are: i) high expense of catalysts; ii) toxicity of transition metals; iii) difficulties in the removal of trace amounts of toxic-metal residues from the desired product; and finally, iv) the large consumption of heavier and rare transition metals which do not meet the requirement of sustainable development. In this regard, developing environmentally benign catalysts is an ideal alternative. Naturally, the most recent trend in catalyst development heralded a new era using either earth-abundant, nontoxic, inexpensive metals or metal-free catalysis. This talk will discuss our recent developments [1-5] on systematically mimicking transition metal-based catalysis using small molecules. In this approach, we have used the smallest polycyclic odd alternant hydrocarbon namely phenalenyl (PLY)-based molecules for designing electron transfer catalysis[1-4] inspired by an entirely different field of molecular spin electronics[2,5].

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Prof. Swadhin K. Mandal is currently a professor at the IISER, Kolkata. He completed his BS and MS studies at the University of Kalyani. Following this, he earned his doctoral degree under the supervision of Prof. S. S. Krishnamurthy at the Indian Institute of Science, Bangalore, in 2002. Subsequently, he has been a postdoctoral fellow at the University of California, Riverside, USA, with Prof. Robert C. Haddon and an Alexander von Humboldt fellow at the University of Göttingen, Germany, with Prof. Herbert W. Roesky. He joined IISER Kolkata in 2007 as an assistant professor. His current research interests include transition metal-free catalysis using reactive main group species and electron transfer catalysis using small molecules in organic transformation, CO_2 fixation and its conversion into value-added chemicals. His research works are documented in various journals (~120 publications and several patents) of high international repute, including Nature, JACS, Angew Chem, Chem Sci, etc.

Prof. Tapas Chakraborty

Ion mobility mass spectrometry

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Mass spectrometry is an indispensable analytical tool in chemical analysis, and allows measurements of molecular masses up to many tens of kilodaltons with high degree of accuracy. Valuable information about the molecular identity including the presence of functional groups and connectivity of the atoms in molecules are also extracted routinely analyzing the MS-MS fragmentation pattern of the molecular ions in the collision cell of a mass spectrometer. However, identification of a completely unknown molecule by means of mass spectrometry alone is still a challenge. Spectroscopic methods, on the other hand, as used in different ranges of the electromagnetic spectrum, are versatile in addressing issues pertaining to molecular structures and conformations. However, as the size of the molecules becomes larger, retrieval of detailed structural information from spectroscopic data are constrained by many factors, and in particular due to spectral broadening, overlap and fast isomeric conversions, in addition to the inherent limitations of the lack of mass selectivity. In my talk, I shall present data from our recent studies to emphasis that much of the desired information pertaining to the structure of a complex molecule can be secured by combining gas-phase ion mobility method with high resolution mass spectrometry and liquid phase chromatography. Measurements of mobility of mass-selected molecular ions through a gas-cell filled with non-interacting gases (helium, nitrogen, carbon dioxide etc.) provide valuable information about global structure of molecules, and much effort has been put to investigate the conformational behavior of large molecules by such means in the recent years [1]. The collision cross-section values as obtained from mobility measurements are now used as molecular markers for different groups of compounds like carbohydrates, peptides, proteins etc. I shall discuss the finding of our recent studies about photochemistry and tautomeric distribution of curcumin, the yellow aromatic dye, the main constituent of turmeric in water-methanol mixtures [2], and also conformational preferences of a popular laser dye molecule (DCM) in methanol solution [3].

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Prof. Tapas Chakraborty, born in the year of 1961 in the Indian state of West Bengal, graduated in chemistry (B.Sc. hons) from Calcutta University in 1985 and continued at the university to complete his master's degree from the university with specialization in physical chemistry. He subsequently enrolled for his doctoral studies on Laser spectroscopy under the supervision of eminent Indian physical chemist, Prof. Mihir Chowdhury at the Indian Association for the Cultivation of Science, Kolkata and after securing a Ph.D. in 1992 from IACS (degree awarded by Jadavpur University), he moved to the US to complete his post-doctoral studies at University of Akron. He completed his postdoctoral studies in 1994 and on his return to India, he joined the IIT Kanpur, where he served as an assistant professor, associate professor and a professor during his stay there from 1994 to 2005; then he continues at IACS as a senior professor at the School of Chemical Sciences, since 2005. During his tenure at IIT Kanpur, he visited Technical University of Munich, Germany as an INSA Visiting scientist in 1997 and also served at Aarhus University, Denmark as visiting professor in 2005. Currently, he is serving as the director of the Indian Association for the Cultivation of Science (IACS) since April 2021.

Prof. Dilip Kumar Maity

Design of Deep Eutectic Solvent with desired properties & validation

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Computational study on a novel deep eutectic solvent (DES) consisting of choline acetate as the hydrogen bond acceptor (HBA) and malonic acid as the hydrogen bond donor (HBD) will be presented. Electronic structure calculations have been performed on a series of HBAs and HBDs, out of which this particular pair with 1:2 eutectic composition found to be best suited to form redox and radiation stable DES. The eutectic composition is predicted from the computed phase diagram. Theoretical results suggest this DES to be more stable than the most popular DES, namely, reline. This is reflected from its huge lowering in melting point indicating formation of strong hydrogen bonds among the components. Experimental results on radiolytic yield of hydrogen shows this DES to be quite stable and comparable to the radiolytic stability of aromatic ionic liquids. The use of choline acetate as HBA in the new DES can open up varied possibilities of its applications starting from enzyme based industrial processes to separation science and technologies.

Prof. Dilip Kumar Maity carried out his doctoral research at IACS, Kolkata. He did his postdoctoral research in Henry Eyring Centre for Theoretical Chemistry, University of Utah, Salt Lake City, USA. He is currently working as Outstanding Scientist in Bhabha Atomic Research Centre, Mumbai. He is a Senior Professor & Associate Dean at Homi Bhabha National Institute, Mumbai. His research interests are in the area of Theoretical & Computational Chemistry. He has extensively worked on hemi bonding and microhydration to understand fundamental processes. At present, he is working on ionic liquids and deep eutectic solvents for various applications. He is a recipient of DAE Homi Bhabha Science & Technology Award, HBNI Distinguished Faculty Award and he is also awarded with Bronze Medal by Chemical Research Society of India. Prof. Maity is a fellow of National Academy of Science India.

Prof. Satrajit Adhikari

Jahn–Teller Effect in Orthorhombic Manganites: Ab Initio Hamiltonian and Roto-vibrational Spectrum

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Optical spectra of $REMnO_3$ (RE = La, Pr, Nd, Sm, Eu, Gd, Tb, Dy) shows anomalous temperature dependence around the Neel temperature. This behavior could be due to Jahn-Teller effect both in ground and excited states. Such observations have been investigated by constructing model [1] as well as *ab initio* [2] based Hamiltonian to interpret the experimental spectra due to the excitations of the quantum rotors. For the latter case (*ab initio* study), we employ three different electronic structure methodologies, namely, CASSCF, RS2c, and MRCI(SD) to construct *ab initio* adiabatic potential energy surfaces (APESs) and nonadiabatic coupling term (NACT) of two electronic states (^5E_g) of MnO_6^{9-} unit, [2] where one La atom is surrounded by eight such units in $LaMnO_3$ crystal. In the roto-vibrational levels of MnO_6^{9-} unit, peak positions obtained from *ab initio* based excited APESs show good agreement with the experimental satellite transitions [3] validating our earlier model results [1]. Alternatively, the effect of the electron–nuclear coupling is explored by computing theoretically "exact" and numerically "accurate" beyond Born–Oppenheimer (BBO) theory based diabatic potential energy surfaces (PESs) of MnO_6^{9-}, where the peak positions of calculated photoelectron (PE) spectra of MnO_6^{10-} unit show good agreement with the higher satellite transitions in the dielectric function spectra of the $LaMnO_3$ complex.

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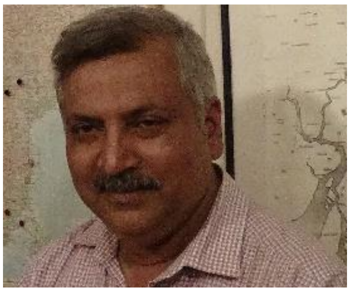

Prof. Satrajit Adhikari is a Senior Professor of Theoretical Chemistry in Indian Association for the Cultivation of Science, Kolkata, India and adjunct Professor at IISER Kolkata. He received his Ph.D. from the Physical Chemistry Department of the same institute. He worked with Professor G. D. Billing for Post-Doctoral research at Copenhagen University, Denmark. Then he served as visiting Scientist at The Fritz Haber Research Center, The Hebrew University, Jerusalem. Currently Professor Adhikari's research focuses on: i) Beyond Born-Oppenheimer theoretical development and its applications on spectroscopic and scattering processes; ii) Methodological development for following the dynamics of multi-electronic multi-mode molecular systems; iii) Thermal effects on molecule-surface scattering; iv) Reaction dynamics for triatomic systems on single (adiabatic) and multiple (diabatic) potential energy surface(s); v) Selective photodissociation dynamics of bonds in small molecules and vi) Role of Jahn-Teller effect in the phase transition of orthorhombic rare earth crystals. He has published close to 151 articles on his areas of research in various international peer-reviewed journals. Professor Adhikari has delivered numerous talks at various national as well as international symposiums and training schools.

Prof. Tarasankar Pal

A galvanic replacement reaction and the Kirkendall effect in the room-temperature synthesis of tubular NiSe₂: a nanozyme catalyst with peroxidase-like activity

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The synthesis of nickel selenide nanostructures under ambient conditions remains fascinating, aesthetically beautiful, and energy efficient, as most reported methods involve high-temperature techniques. In this work, we have reported the wet chemical synthesis of $NiSe_2$ nanostructures at room temperature. The approach starts with nickel nanowires (NiNW) and selenous acid as active ingredients. Upon the incubation of NiNW in selenous acid, zero-valent metallic nickel gradually oxidised with the successive deposition of nano-selenium, a reductive product, over the pristine NiNW surface. This thermodynamically controlled galvanic replacement reaction (GRR) is favourably governed by the reduction potential values of the Ni^{2+}/Ni and SeO_3^{2-}/Se redox couples. Moreover, the selenium nanoparticles over the NiNW surface and the oxidized Ni^{2+} underneath then interplay during inward and outward diffusion. The different diffusivities of the elements/ions cause the generation of void interiors, thus resulting in tubular nanostructures. Therefore, both the GRR and nanoscale Kirkendall effect jointly remain engaged, resulting in the formation of hollow $NiSe_2$ nanotubular structures. Then, we ably exploit this heterogeneous chalcogenide nanostructure material as an artificial enzyme for peroxidase mimics. This provides a method for the naked-eye detection of peroxide in solution. The peroxidase activity was selectively restrained in the presence of glutathione. Hence, a colorimetric assay was simultaneously developed for the selective detection of this biothiol. The intrinsic nanozyme activity of the substrate is hitherto unknown and can, hence, be explored further with other nanostructured nickel selenide materials.

Professor Tarasankar Pal, MSc, PhD, DSc, FNASc, FWAST an alumnus of the University of Burdwan, worked in the Department of Chemistry, IIT Kharagpur since 1984 till 2017. He has highest number of published papers (358) from the department as on today. American Chemical Society configured him from IIT Kharagpur among the top 20 Indian chemistry researchers for high-quality original research activity just before his superannuation. Scopus has identified top three Indian Material Scientists and Professor Pal is among them. He initiated nanoparticle research in India way back in 1983 (Inorg. Chim. Acta, 79B, 283, **1983**). His 'arsenic detection kit' for arsenic affected rural people (Analytical Proceedings 32, 369, **1995 of the Royal Society of Chemistry**) and 'bench marked model reaction' to test any metal nanoparticle catalyst (Chem. Commun., 51, 9410, **2015**) deserve special mention. His research interest includes inorganic chemistry (reported 1st inorganic gel in Chem. Commun**.,** 49**,** 9428**, 2013**), synthesis and applications of metal and semiconductor nanoparticles for catalytic, photocatalytic, electrocatalytic and spectroscopic applications. Original contribution to Surface-enhanced Raman scattering (SERS), synergistic fluorescence enhancement by Ag and Au particles and supercapacitor fields are noteworthy. Prof. Pal has received numerous National and International Awards which include INSA Royal Society Exchange Fellowship, ISCAS Gold Medal, Prof. J N Mukherjee endowment Gold Medal, R & D-100 Award from the U.S.A, CRSI medal etc. He has received President Award from the Tokyo University of Science, Japan and selected as a 'Visiting Researcher' for science without border programme, UFSC, Brazil. He has visited USA, UK, Germany, Italy France, Japan, China, Taiwan, Singapore, Mexico, Brazil as a 'Visiting Professor. Professor Pal has supervised a good number (32) of students for their PhD degree and most of them are established scientists. Now he is a Distinguished Visiting Professor in the University of Johannesburg, South Africa. World ranking placed him among the top 2% scientists. In 2022 he has been placed as the best scientist of IIT Kharagpur.

Dr. Ranganathan Subramanian

Molecular Clusters of water with implications in atmospheric chemistry, and cooperativity of hydrogen bonds

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The atmospheric new particle formation (NPF) creates secondary aerosols from gaseous vapors that go through gas-to-particle (GTP) conversion. We have used water clusters to investigate the principles of intermolecular interactions, including the formation of hydrogen bonds and cluster structure, as well as phenomena like solvation and nucleation that are important to atmospheric transitions from the gas phase to clusters to aerosol particles. We will discuss water clusters of Sodium-ion (Na^+), Methanol, Ethanol, and Formic acid. We have used DFT methods to investigate the water clusters and to obtain a physical interpretation of the interaction energy with descriptions obtained for several energy terms utilizing the SAPT method. The clusters are studied using the quantum theory of atoms in molecules to understand cooperativity in hydrogen-bonded interactions to obtain a meaningful understanding of cooperativity in hydrogen-bonded interactions.

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Dr. Ranganathan (Ranga) Subramanian is working as an Associate Professor in the Department of Chemistry, IIT Patna, and obtained his Ph. D. from Wesleyan University, Middletown, CT, in 2003. He was a postdoctoral fellow in the Department of Chemistry, University of Arizona and Tulane University, USA. He worked as a Visiting Assistant Professor at New College of Florida, USA. Dr. Ranga's research revolves around Computational Chemistry, Gas Phase Molecular Spectroscopy. His group is presently studying ab initio studies applied to Atmospheric Science. In the last decade, we have looked at reactions of radicals with molecules with atmospheric interest. We have recently been exploring atmospheric new particle formation, especially with water.

Prof. Sukhendu Nath

BODIPY dyes for the detection of protein fibrils and protofibrils

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Aggregation of protein to form amyloid fibrils under physiological stress is responsible for several neurological diseases. Efforts are being given for the selective and sensitive detection of these protein aggregates. Several classes of organic molecules have been explored as amyloid probes. Among others, BODIPY dyes are very promising as amyloid probes due to their emission in the red region and extreme photostability. BODIPY dyes are also explored extensively due to the flexibility in their synthesis and tunability in their photophysical properties. We have synthesized three BODIPY dyes and explored their use as fluorescent probes for amyloids. A correlation between the molecular structure of these BODIPY dyes and their amyloid sensing capacity has been established. Further, one of the BODIPY derivatives has shown promise to detect protofibrils which are otherwise difficult to detect. Detailed photophysical properties of these three BODIPY dyes will be presented.

Prof. Sukhendu Nath completed his graduation and post-graduation from University of Burdwan. He joined BARC in 1996 and completed his Ph.D. from University of Bombay. He did his postdoctoral research in University of South Carolina. He is currently heading the ultrafast spectroscopy group in BARC. His research interests are ultrafast dynamics, biosensor, supramolecular assemblies and multi-dimensional vibrational spectroscopy. He was awarded INSA Young Scientist Award, Science and Technology Excellence Award by DAE and Distinguished Lectureship Award by Chemical Society of Japan.

Dr. Saptarshi Mukherjee

Designing an Artificial Light Harvesting System and Monitoring Conformational Dynamics of i-motif DNA Using Förster Resonance Energy Transfer

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Dipole-dipole interaction among chromophores facilitates the transfer of excited state energy to the other chromophore: a phenomenon popularly known as Förster Resonance Energy Transfer (FRET).[1] This purely non-radiative energy transfer is governed by the distance (2-10 nm) between the FRET pair, and hence, it is referred to as "spectroscopic nanoruler".[1] Being a sensitive fluorescence technique, it has occupied the central stage in the field of biophysical studies, nanoscience, material science and several interdisciplinary research. FRET is also extensively employed to a wide variety of systems ranging from designing artificial bioinspired light harvesting system (LHS) to investigate the conformational dynamics of intercalative-motif (i-motif) DNA. Nature has beautifully assembled its light harvesting pigments within the protein scaffolds that ensures a very high energy transfer.[2] Motivated by nature's own architecture for light harvesting complexes, a highly efficient artificial LHS is generated using a self-assembled nanostructure of a homopolypetide (poly-D-lysine, PDL) making use of their β-sheet structure in aqueous solution.[3] Such homogeneous β-sheet structure acts as an assembly hub to align two chromophores in close proximity. The chromophores used are compatible for a highly efficient energy transfer process, are non-fluorescent in aqueous medium but exhibit high fluorescence intensity when bound to the nanostructure of PDL and generates white light emission. On the other hand, the effect of confinement on folding pathway of noncanonical (i-motif) DNA under physiological condition is extensively studied by single-molecule FRET (smFRET).[4] Such kind of noncanonical DNA has been considered as a novel drug target in the field of anticancer research.[5] Hence, it is pertinent to have a better understanding as to how various drugs interact with the highly dynamic structures of noncanonical DNA. In view of this, a detailed illustration of the structural dynamics of *c-MYC* promoter-based i-motif conformation has been investigated at physiological condition within a microemulsions having various nanodimensions. It is concluded that the folding of such motifs under cellular-like confined environment is not a direct transition between unstructured random coil to a structured i-motif, rather it occurs through a partially folded intermediate depending, on the confined dimension.[4]

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Dr. Saptarshi Mukherjee is presently a Professor at the Department of Chemistry, Indian Institute of Science Education and Research (IISER) Bhopal. He did both his BSc and MSc from the Jadavpur University and carried out his doctoral research at the Indian Association for the Cultivation of Science, Kolkata under Professor Kankan Bhattacharyya on Time-Resolved Laser Spectroscopy. He then moved to the Bowling Green State University, Ohio for his post-doctoral research with Professor H. Peter Lu on Single Molecule Spectroscopy. He returned to India in late 2008 and joined the Department of Chemistry IISER Bhopal as an Assistant Professor where he still continuing.

Professor Mukherjee's research interests include ultrafast and single molecule spectroscopy of luminescent metal nanoclusters and self-assembled systems having biological relevance. He is the recipient of the INSA Young Scientist Award, CRSI Young Scientist Award, CRSI Bronze Medal and has been a Core and Founding Member of Indian National Young Academy of Sciences (INYAS). Professor Mukherjee is a Fellow of the National Academy of Sciences, Allahabad and is a Senior Editor of Chemical Physics Impact, a journal published by Elsevier. He has also served IISER Bhopal as its first Deputy Director.

Dr. Sujit Kumar Ghosh

Solvent and Ligand Dielectric Sensitivity of the Optical Properties of Metallic Nanostructures

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The brilliant colors of the dispersions of metallic colloids have been fascinated since antiquity, long before our understanding of light-matter interaction. The ability of noble metal colloids to manipulate light at the nanoscale has pioneered an emerging research area called plasmonics. The physical origin of the light absorption by metal nanoparticles is the coherent oscillation of the conduction band electrons, coined as, localized surface plasmon resonance (LSPR). The resonance frequency of this LSPR is strongly dependent upon the size, shape, interparticle interactions, dielectric properties, and local environment of the nanoparticles. As in many disciplines of fundamental physics, chemistry and biology, the past two centuries have made significant contribution in the investigation of optical phenomena at the nanometer scale pioneered by specific theoretical approaches to solve Maxwell's equations, together with powerful simulation techniques that are able to anticipate experimental observations. In this presentation, the localized surface plasmon sensitivity of metallic nanostructures towards the local dielectric environment and their plausible applications will be elucidated.

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Dr. Sujit Kumar Ghosh being graduated from Indian Institute of Technology, Kharagpur in 2005 working under the supervision of Professor Tarasankar Pal, served as a Lecturer in Chemistry at Raidighi College for a couple of years. He was a Postdoctoral Research Associate at Tokyo University of Science at Yamaguchi, Japan and Alexander-von-Humboldt Fellow at RWTH Aachen University, Germany. Since 2010, he was serving as Assistant Professor at the Department of Chemistry, Assam University, Silchar. This year, he has joined as Associate Professor at the Department of Chemistry, Jadavpur University, Kolkata. He has published 113 articles in national and international journals of repute. His current research interest includes on the plasmonic properties of metal nanostructures, photophysical aspects of molecular probes on the surface of nanoscale materials and correlation between plasmonics and thermodynamics at the nanoscale.

Dr. Sumanta Bhattacharya

Photophysical Insights on Energy Transfer Phenomena in Quantum Dots-Tetrapyrrole System in Solution

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The distinct physical properties of quantum dots (QD), such as, large extinction coefficients, size-dependent electronic structure, and multiple exciton generation acquiesces them exquisite candidates as photon harvesters [1]. On the other hand, the nanometric dimensions of tetrapyrrole macrocycle, e.g, porphyrin and porphyrazine (a typical tetraphenylporphyrin is of 1–2 nm in diameter) makes them ideal for investigations that include complex nanostructures and are among the most stable of common organic molecules, even capable of surviving conditions under which semiconductor silicon is normally processed [2]. Combination of QD with porphyrin and porphyrazine allows greater flexibility to form QD-porphyrin and QD-porphyrazine hybrid systems, respectively, with photoinduced energy transfer properties. The present research focuses in understanding the photophysical insights and chemical physics on interaction of QD with tetrapyrrole macrocycle (i.e., porphyrin and porphyrazine) in solution [3-7]. The above studies envisage that QD-porphyrin and QD-porphyrazine systems would lead to very good perspective for the development of efficient photochromic devices in near future.

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Dr. Sumanta Bhattacharya has obtained his Ph.D. degree in Science (Chemistry) in 2003 from The University of Burdwan and continued his research as a Research Associate of CSIR in same University. He then moved to Shiga University of Medical Science, Japan as a JSPS post-doctoral research fellow in 2005. After spending near about two years in Japan, he joined IIT Guwahati as an Assistant Professor in Chemistry in March 2007. In September 2007, he returned to The University of Burdwan as a faculty in Chemistry. He became Professor in Chemistry in 2013 and continuing his job in the same rank till date. Dr. Bhattacharya won several Honors and distinctions including S. R. Palit award from Indian Chemical Society in 2003, DST FAST TRACK Research Award in 2007, DAE Young Scientist Research Award in 2010, UGC Research Award in 2014 and William J. Acree award from COGNIZURE in 2015 for outstanding research in Physical Chemistry. He was selected as member in National Academy of Sciences India in 2021. Till date, he has delivered more than 30 numbers of invited talks in various International and National Conferences, Refresher Courses and Orientation Programme. Apart from this, he has successfully completed eight numbers of research projects under DST, DAE, CSIR, WB-DST and UGC, New Delhi and now guiding one research projects under CSIR scheme. Till date, six numbers of research students have earned their Ph.D. degree under his supervision, two candidates performed post-doctoral research work and two numbers of research scholars are now doing their Ph.D. and Post-Doctoral work under his guidance. He has published more than 115 numbers of original research papers in journals of very high international repute like Nature Nanotechnology, Chemical Communications, Journal of Physical Chemistry A & B, Chemical Physics Letters, Journal of Molecular Liquids, RSC Advances, Spectrochimica Acta Part A etc. His current research interests are “Supramolecular Photochemistry of Fullerenes and Functionalized Fullerenes with Porphyrinoids and other macrocyclic receptors in solution” and “Photophysical insights on Quantum Dot-Dye interaction in solution”.

Dr. Kalluri V.S. Ranganath

Chiral Surfactant Stabilized Nanoparticles: Characterization and application in Catalysis

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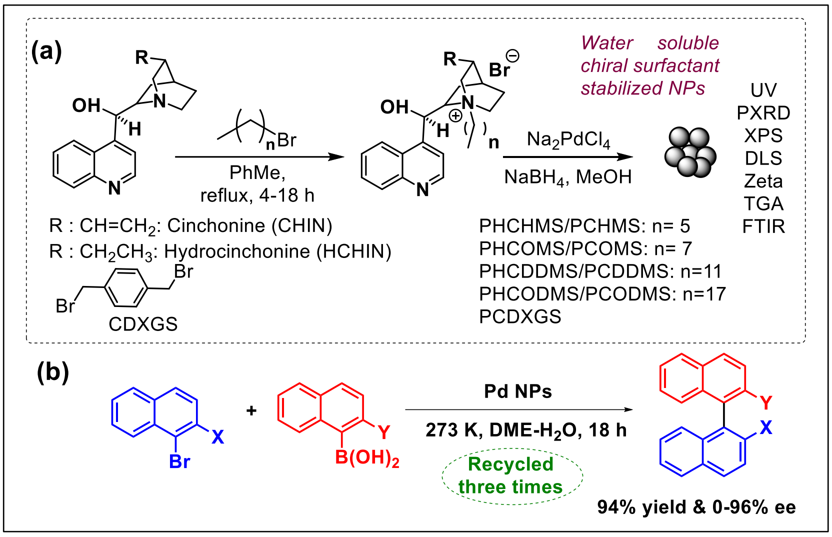
Surfactant stabilized nanoparticles have their own importance in catalysis because of their inherent properties associated with them such as high surface area. Chiral surfactants stabilized Pd, Pt, Rh and Ru NPs are widely used in various asymmetric catalysis. We prepared cinchonine based surfactants by reacting with various alkyl bromides such as hexyl, octyl, dodecyl and octadecyl. These chiral surfactants are well characterized by UV, DLS, Zeta Potential, XPS and PXRD measurements. The use of NPs as effective active species in asymmetric process remains challenge. In this, we would like to discuss the synthesis of chiral surfactant stabilized palladium NPs and their catalytic application in asymmetric Suzuki cross coupling reactions (Scheme 1).



Scheme 1. a) Synthesis of Pd NPs stabilized by chiral mono and gemini surfactants b) Asymmetric Suzuki coupling reaction of naphthalenes catalyzed by Pd NPs

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Kalluri V.S. Ranganath received his B.Sc from Nagarjuna University, Guntur and M.Sc in physical chemistry from S.V University, Tirupati. Later, he completed his Ph.D from IICT, Hyderabad under the supervision of Prof. B.M. Choudary on nano catalysis. Thereafter he did postdoctoral studies in Japan with Prof. Junji Inanaga as a JSPS fellow on self-organized materials for catalysis. Later he was offered an AvH postdoctoral fellowship with his research proposal on asymmetric catalysis using N-heterocyclic carbenes as chiral modifiers with Prof. Frank Glorius. Dr. Ranganath was awarded DST-Ramanujam fellowship in 2012. Currently he is working as a Professor in Physical Chemistry at Banaras Hindu University, Varanasi. His wide research areas include asymmetric catalysis, development of new materials for the synthesis of furan derivatives and polymers.

Prof. Debashree Ghosh

Photophysics of skin pigment melanin

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The biological pigment melanin is the primary component in our skin that is responsible for photoprotection from sunlight. While this fact is well acknowledged, the exact molecular mechanism of the process is much more obscure. It is further complicated because of the lack of knowledge about the exact structure of melanin. We use computational tools to understand the mechanism of photoprotection in melanin [1,2] and find the crucial role of heterogeneity is central to efficient nonradiative decay without any structural damage. [3] To understand such processes we develop methods that are capable to deal with strongly correlated systems, such as density matrix renormalization group. [4-6]

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Prof. Debashree Ghosh studied chemistry and obtained her B.Sc. in Chemistry from Presidency College, Kolkata in 2002, her M.S. degree in Chemical Sciences from Indian Institute of Science, Bangalore in 2005. She did her PhD at Chemistry and Chemical Biology department in Cornell University, USA under the supervision of Prof. Garnet K.-L. Chan. She did her postdoctoral training from University of Southern California with Prof. Anna Krylov. She joined CSIR-National Chemical Laboratory as a Senior Scientist in 2012, subsequently moving to Indian Association for the Cultivation of Science. Currently she is a professor at IACS. Her current research focuses on the development of polarizable force fields and their hybrid frameworks with excited-state electronic structure methods for the understanding of solvent effects on the spectra of biological systems. She is also the Associate Editor of Royal Society Open Science and serves in the Editorial Boards of International Journal of Quantum Chemistry, Physical Chemistry Chemical Physics, Electronic Structure, Molecular Physics and Journal of Chemical Sciences.

Dr. Debashis Panda

Continuous Making and Light Harvesting of Organic Nano-Tetrahedrons

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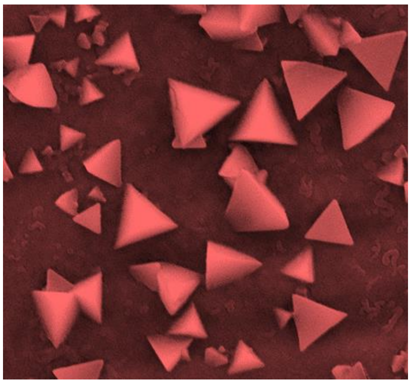
There is a global hunt for photoluminescent organic nanocrystals. And in the last decade extensive research was carried out on Carbon Nanodot. In this talk, I will share with you the debate and progress made to unearth Carbon Nanodot. The scientific community is divided between two orthogonal views- a material perspective and a spectroscopist perspective. How can we correlate the images in HRTEM (solid phase) with Photoluminescence in water? In summary, what we understood is that carbon nanodot is nothing but organic fluorophores. We have used flow chemistry (coiled flow reactor) to synthesize the organic fluorophores often termed carbon nanodot in real-time. The organic emitters are found to be stimuli-responsive in nature, even upon aggregation, these molecular fluorophores transform into nano-sized organic tetrahedrons (3-sided pyramid) that show remarkable emission characteristics and photocatalytic properties.



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Debashis Panda received his B.Sc. from Calcutta University (Ramakrishna Mission Residential College, Narendrapur), and M.Sc. and Ph.D. from IIT Bombay. In his postdoctoral research he worked with Prof. Peng Chen at Cornell University, New York on single-molecule fluorescence spectroscopy and with Late Prof. Kazuhiko Kinosita Jr at Waseda University, Japan on Single-molecule biophysics. He was also offered JSPS-postdoctoral fellowship for his research proposal with Prof. Tetsuro Majima, Osaka University, Japan. He was awarded DST-SERB Young Scientist in 2014. Dr. Panda joined Rajiv Gandhi Institute of Petroleum Technology, An Institution of National Importance, Govt. of India and is currently serving as an Associate Professor there. His diversified research interests include- Luminescent Nanostructures, In-operando Nanocatalysis, Valorization of Rice-Straw and Flow Chemistry. His overarching research goal is to produce hydrogen from rice-straw using photo-thermo-catalytic route.

Dr. Manmohan L. Satnami

Carbon Quantum Dots: Photoluminescence Properties and FRET Donor Efficiency

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Carbon quantum dots (CQDs) are a new class of fluorescent carbon nanomaterials with particle size of less than 10 nm, and received extensive attentions from its first discovery in 2004 during purification of single-walled carbon nanotubes (SWCNTs).[1] A large number of investigations on CQDs in last two decades are due to their strong and tunable fluorescence (FL) properties, which enable their applications in sensing, catalysis, biomedicine, optoelectronic, and bioimaging.[2] The effect of heteroatom doping, enhanced quantum yields (QYs), and fluorescence mechanism such as quantum confinement, surface state and molecular fluorophores have largely been debated. The nature of doping of nitrogen atoms such as graphitic, pyridinic, pyrrolic and amine plays significant roles in modulating the fluorescence QYs, energy levels and fluorescence decay life time of CQDs.[3] Synthesis of multicolor emissive CQDs can meet the current challenge of new LED materials. The fluorescence quenching (Turn-off) and fluorescence recovery (Turn-on) properties can be used for sensing large class of analytes of environmental and biological importance. The fluorescence tunability of CQDs make them suitable donors for fluorescence resonance energy transfer (FRET) with wide range of donor materials. Due to significant overlapping of FL spectra of CQDs with absorption spectra of gold nanoparticles (AuNPs) and mangnese dioxide (MnO_2) nanostructures, we enabled to develop FRET based sensors for detection of pesticides and biomolecules such as glutathione, cholesterol and acetylcholinesterase (AChE) enzyme.[4-5] Owing to aspect ratio, gold nanorods (AuNRs) showed short wavelength transverse and long wavelength longitudinal absorption. The FRET between carbon quantum dots (CQDs) and AuNRs may arise from distinctive overlap of transverse and longitudinal bands of AuNRs with fluorescence (FL) spectra of CQDs. In this context, we have developed a FRET based probe for the detection of glucose, glutathione and acetylcholinestrase enzyme. A series of nitrogen-doped carbon quantum dots (Blue, Green, Orange and Red) were synthesized by hydrothermal method. The fluorescence resonance energy transfer (FRET) based fluorescence "switch-off-on" of N-CQDs (energy donor) in presence of gold nanorods (energy acceptor) has been successfully applied to fabricate a fluorometric sensor for the detection purpose.

Keywords: Carbon Quantum Dots, Photoluminescence, FRET, Sensors

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Dr. Manmohan L. Satnami is currently working as Associate Professor in school of studies in chemistry, Pt. Ravishankar Shukla University, Raipur (Chhattisgarh). Dr. Satnami obtained his Ph.D. degree from same institution under supervision of Prof. Kallol K. Ghosh in 2007, and then worked as a postdoctoral fellow at department of chemistry, Federal University of Santa Catarina, Florianopolis (SC), Brazil under the TWAS fellowship scheme. He has been awarded with TWAS-CNPq postdoctroal fellowship (2007-2008), DST young Scientist (Fast-Track 2012-2015), UGC research award (2016-2018), CRSI young scientist award (2018), and best teacher award of Pt. Ravishankar Shukla University (2015). He has published more than 65 research papers, and delivered more than 20 talks in different scientific programs. His personal academic h index is 26. Dr. Satnami has made original contribution to the nanomaretial-based sensors for detection of pesticides and biological molecules in environmental and biological matrix. His research interest includes synthesis, characterization of nanomaterails such as metallic nanoparticles, quantum dot nanocrystals, carbon quantum dots, and their sensing applications. So far 6 (six) students have been awarded with Ph.D. degree and 10 (ten) students have completed their M. Phil. dissertation under his supervision. He has completed 4 research projects funded by DST, SERB, UGC and CCOST, Raipur. He has visited Brazil, Argentina, Malaysia for academic presentations.

Dr. Sudipta Seal

Designing Nanoceria: Biomedical Applications

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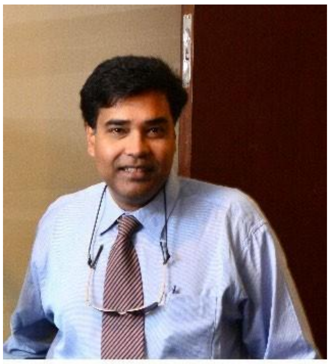
Oxidative stress, the excessive generation of reactive oxygen species (ROS) and reactive nitrogen species (RNS), respectively, hinder the normal functioning and induces damaging effect to the cellular machinery. Specially formulated nanoceria mimics the catalytic properties of antioxidative enzymes and induces protective effect through regenerative scavenging potential and ameliorates the disease states further. Based on its design methodology, nanoceria has been developed for scavenging of different toxicROS and RNS molecules including superoxide anions, hydrogen peroxide. Nanoceria has been found to accelerate the wound healing process through reducing the oxidative/nitrosative damage and inducing proliferative effect on the migration of keratinocytes, fibroblast and vascular endothelial cells. Further, nanoceria's regenerative properties was also explored for coating of metal implants with SOD/Catalase mimetic activity to prevent osteolysis.



Sudipta Seal, FASM, University Distinguished Professor, Trustee Chair and UCF Pegasus Professor, joined University of Central Florida (UCF) in fall 1997 after a postdoctoral work at Lawrence Berkeley National Laboratory, University of California, Berkeley. At UCF, he pioneered nanostructured cerium oxide and other metal/oxide platforms (micro to nano), discovered its antioxidant properties, and applied in various biomedical problems. He served as a Director of Advanced Materials Processing Analysis Center, and Nanotechnology Center, currently Chair of newly created Materials Science and Engineering and holds an appointment with College of Medicine. He is the recipient of the 2002: Office of Naval Research Young Investigator Award (ONR-YIP), JSPS fellowship, Alexander Von Humboldt Fellow, ASM IIM Lecturer award, Royal Soc of Eng - Visiting Professor Distinguished Fellowship at Imperial College, UK, etc. He was elected to attend the Frontiers of Eng Symposium by National Academy of Engineering. He is the recipient of Fellow of FASM, FAAAS, FAVS, FIoN, FAIMBE, FNAI, FECS, FMRS, FRSC, FACERS. He is inducted the Florida Hall of Fame of Inventors, elected World Academy Ceramics Academician, recently inducted to Florida Academy of Science, Engineering & Medicine. He has more than 400 journal papers, books and h index> 104. He has more than 85 issued patents and his technology is responsible for various startups.

Catalytic activity and Physico-Chemical Properties of Ln_2M0_4 type NON-Stiochiometric oxides of Praseodymium with Cobalt and Nickel

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Abstract:

AB_2O_4 Spinel type of non-stoichiomertic oxides of Praseodymium with Cobalt and Nickel were synthesized by solid state reaction technique at 973,1073,1173 and 1273 K for 18 hrs.in lack of oxygen . AB_2O_4 type of d Spine belong to cubic space group $o^7{}_8$ with eight oxygen molecules in the unit cell. A atoms on octahedral sites of D_3d symmetry and B atoms on tetrahedral sites of T_4 symmetry[1] .] Different surface properties like surface area , surface acidity , excess surface oxygen and activation energy and activation energy were measured by reported methods[3-].]

The decomposition of urea in presence of different oxide catalysts was performed to describe the catalytic property of these oxides at 413,423 and 433 K. Nickel containing oxides were found a bit more Catalytic active in comparison to the cobalt containing oxide samples.

Characterization of different spinel oxides samples was done by XRD and FTIR methods. the XRD data for each sample was analyzed through a standard computer programme called "Powdmult" and best structural information derived was as follows for one of the sample pr_2NiO_4 prepared at 1073 K.

$a= 10.0819^0$ A , $b=9.6614^0$ A , $c = 8.9125^0$ A , V = 625.94 showing that all spinel samples have orthorhombic structure . The appearance of diffractions suggested good crystallinity of oxide samples mostly found in single phase . The IR spectra corresponding to the same sample prepared at 1013 K has been described .Its symmetry predicts four infrared vibrations V_1,V_2,V_3 and V_4 . The vibration v_1 is sensitive to the change in interaction between oxygen and cations and these are frequently present in the wave number 418 to 653 cm^{-1} in all cases which corresponds to spinel structure[14-16] . our measurement of the spectrum of the powdered sample yielded the band, which is also in good agreement with the reported[18] value of single crystal.

The rate constants of the urea degradation reaction catalyzed by samples were calculated from the inital slopes of the rate curves-log ($v^{\infty}{}_{-\ Vt)\ Vs}$ s t (time).

the most interesting non -stoichiometric oxides are found in transition metal and rare earth oxides at higher temperatures. These oxdies have been the subject of intensive investigations because of their interesting catalytic, electrical and magnetic properties[2-5] and have wide applications in petrochemical, fertilizer, pharmaceutical and food -stuff industries.

Development of UCNPs Embedded Functionalized POP for NIR triggered Chemo and Photodynamic Therapy

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Abstract:

Multifunctional nanomaterials with surface functionality, high loading capability along with excellent property to generate reactive oxygen species (ROS) upon photoexcitation have attracted much attention in recent years for diagnosis and therapy of cancer. (1, 2) In this work, we have synthesized folic acid (FA) encapsulated upconversion nanoparticle@Porus Organic Polymer (UCNPs@POP/FA) composite for cell imaging, targeted drug delivery and photodynamic therapy. Here, PEI-coated upconversion nanoparticle is selected for NIR mode imaging as well as FRET donor. (3) -COOH functionalized POP is synthesized with UCNPs in one step to achieve high porosity and surface area. NH2 functionalized Folic acid is attached with the composite to avail cancer targeting efficiency. Subsequently, high amount of anticancer drug doxorubicin hydrochloride (DOX) is loaded into the composite UCNPs@POP/FA and the composite shows targeted drug delivery as well as pH-responsive drug release to treat cancer. Moreover, singlet oxygen generation occurs after the loading of methylene blue (MB) photosensitizer followed by irradiation with 980 nm via FRET from UCNPs to MB. The composite shows A549 lung cancer cell destruction by intracellular ROS generation.

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Functionalized Eco-friendly Magnetite Nanoparticle Decorated on Nontoxic MoS2 Nanosheet Biosensor for Investigation of Hazardous 4-Aminoantipyrine

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Abstract:

4-Aminoantipyrine (AAP) is hardly administered as an analgesic drug because of severe side effects. The residue of AAP in the environment is potentially harmful. The primary focus is on examining AAP in biological and environmental samples. A novel AAP sensor is being developed using Hydrocerol A coated green magnetite nanoparticles decorated MoS2 nanocomposite modified glassy carbon electrode (HCA-Fe3O4/MoS2@GCE). Using the SWV technique in pH 3.0 phosphate buffer, the examination of samples of blood, urine and water spiked with AAP was monitored. The limit of detection and quantification is found to be 9.8nM and 30 nM respectively. The electrode material was characterized by CV, scanning electron microscopy (SEM), atomic force microscope (AFM), and electrochemical impedance spectroscopy. A suitable mechanism was proposed for the electro-oxidation of AAP.

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Understanding the effect of the surroundings on the aggregation behaviour of a substituted phenol

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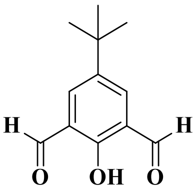

Figure 1. Molecular structure of 5-(tert-Butyl)-2-hydroxyisophthalaldehyde (5-tBHI)

5-(tert-Butyl)-2-hydroxyisophthalaldehyde (5-tBHI) is a common precursor to synthesize a variety of fluorescent probes.[1-2] 5-tBHI, having a π-conjugated planar structure like benzene, is susceptible for π-π stacking.[3] This intrigued us towards understanding its photophysics, which is still unexplored. From the steady state as well as time resolved absorption and emission spectra of 5-tBHI, it is found that there is a dynamic equilibrium of 5-tBHI monomer and its aggregates of different order, subject to concentration of the probe as well as solvent polarity and pH. The aggregates are found to be H*-aggregates in nature and are less emissive with respect to the monomer. The spectroscopic data are supported by the SEM and FLIM images.

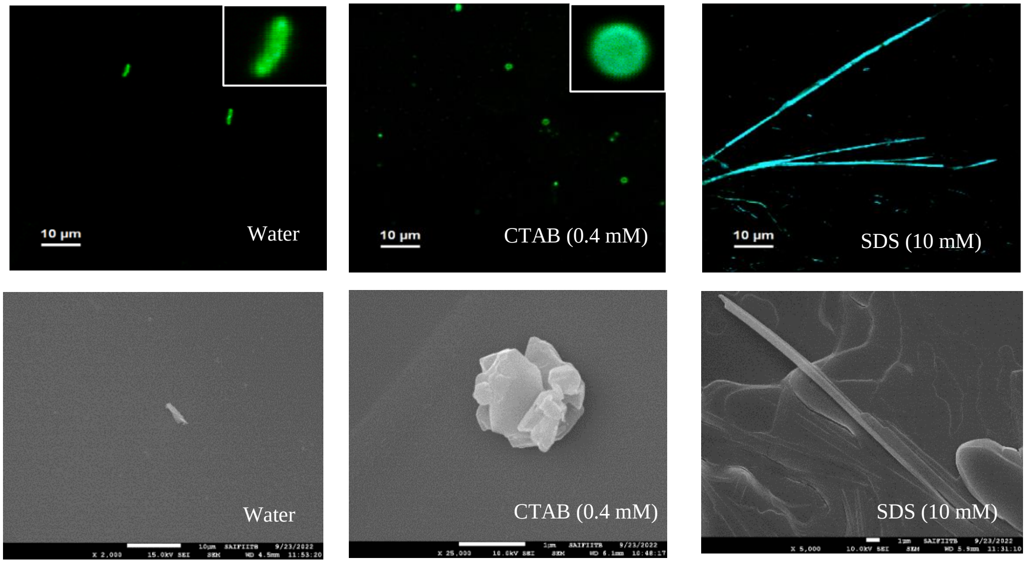

Figure 2. FLIM (top row) and SEM (bottom row) images of 10 µM of 5-tBHI in water, 0.4 mM CTAB and 10 mM SDS respectively.

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In Situ Chemical Synthesis of g-C3N4/In2O3 Semiconductor Composites for Photoelectrochemical Water Oxidation

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Abstract:

This work reports the heat-treatment method to obtain g-C3N4/In2O3 composite semiconductor following deposition-precipitation technique. The photoelectrochemical results showed that the composite semiconductor's properties were much superior to pristine g-C3N4 or In2O3. The optimized 5.0 wt% g-C3N4/In2O3 composite shows the best photocurrent output of 1.3 mA cm–2 at 1.2 V vs Ag/AgCl for water oxidation. The electrochemical impedance spectroscopic Mott-Schottky analysis indicates n-type semiconductivity of the as-prepared composites. The electrochemical action spectra show ~48% incident photon to current conversion efficiency for the optimized photoanode. The photocatalytic properties had been assessed through degradation of methylene blue (MB), which follows first-order kinetics. The photodegradation rate constant of MB for g-C3N4 (5.0 wt%)/ In2O3 is 0.0190 min–1, which is almost doubled as compared to pristine In2O3 (rate constant: 0.0110min–1). The improved PEC performances derived from the transport of excited electrons from the conduction band of g-C3N4 to In2O3.

Keywords: graphitic-C3N4; Indium oxide semiconductor; in-situ chemical synthesis; PEC activity; charge carrier separation; electrochemical characterizations.

Escalation of Photoelectrochemical response of WO3 Semiconductor through judicious insertion of Ca & study of photocatalytic activity

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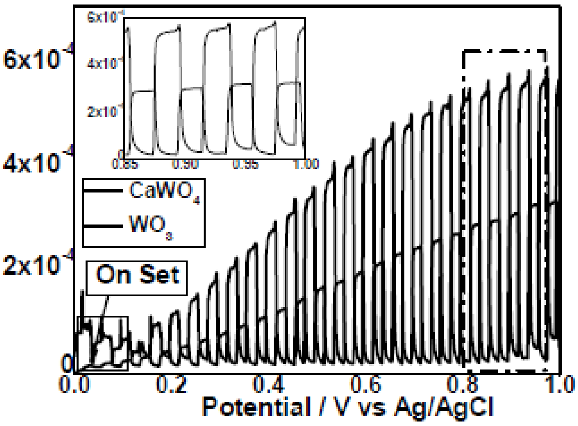
Abstract:
Semiconductor/electrolyte interface are considered the most promising technique to harness solar energy to hydrogen economy by splitting H2O to meet the concern of the global energy crisis. In the present study drop-cast method was employed to fabricate the Ca-modified WO3 semiconductors on FTO-coated glass substrates. The bandgap energy of 2.6 eV was determined through absorption spectra whereas, SEM & XRD analysis confirms the distinct morphological change and scheelite crystallites of pure and @ Ca inserted tungsten oxide, respectively. The photoelectrochemical activity of SC having composition Ca:W 1:9 (V/V) exhibits 1.5 times higher photo-current (510 µA/cm2) compared to the pure WO3 (270 µA/cm2) under 100 mW/cm^2 illumination. The Nyquist analysis shows lower charge transfer resistance for Ca-modified WO3. The photocatalytic study is done by monitoring the deterioration of more than 85% methylene blue in just 40 min of illumination as water pollutant.



Keywords: Calcium tungstate, n-type semiconductor, photoelectrochemical water oxidation photocatalytic activity.

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Rab$_2$B in Cell Mimicking Environment: A Biophysical Perspective

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Abstract:

Rab2B which belongs to the RAS superfamily controls vesicular trafficking between various subcellular compartments within eukaryotic cells. Small GTPase Rab2 is a resident of pre-golgi intermediates and is required for protein transport from the Endoplasmic Reticulum to the Golgi complex .Two Rab2 genes (Rab2A and Rab2B) have been identified in human genome, with 82% protein sequence identity. It has been proposed that Rab2B has a close relationship with colon tumors. This is different from Rab2a which is associated with neoplastic diseases during immunological events.These proteins act as molecular switches between a GDP-bound inactive form and GTP-bound active form in which they recruit downstream effectors onto membranes. On the other hand, the intracellular environment is a rather crowded one with the concentration reaching values as high as 400 g/L and that too in an organelle dependent fashion, with the ER and Golgi typically having a very high local density of macromolecules. Thus, keeping the importance of Rab2B in mind and the crowded milieu it carries out its functions in presence of, our present work focuses on biophysical studies of the protein in cell-mimicking environments. Two of the mostly commonly used macromolecular crowders, Ficoll 70 and PEG 8000, have been used and their influence on the conformational properties of Rab2B (recombinantly expressed and purified) studied. The data obtained thus far show significant modulations of the structure and conformation of Rab2B in the crowded milieu.

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How promising is Lithium Fluoride (LiF) as a hydrogen storage material?

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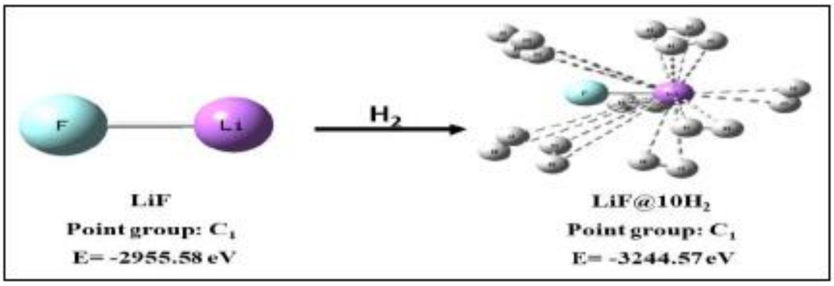
Keywords: Binding Energy, Quasi-molecular Adsorption, Gravimetric wt%.

Abstract:

The LiF molecule has been identified as a promising hydrogen storage material since the average adsorption energy per H2 molecule supports a quasi-molecular adsorption process. According to the NBO analysis, the charge on the Li atom progressively drops with the gradual increase of H2 adsorptions, indicating that a charge transfer interaction occurs between the bonding orbitals of H2 molecules and the antibonding orbitals of Li.1 A single LiF molecule can adsorb up to 10 H2 (LiF@10H2) with a high gravimetric wt% value (43.48). The amazing results demonstrate the LiF molecule as a promising hydrogen storage material w.r.t U.S.D.O.E. standards. According to the atoms in molecule (AIM) analysis, molecular hydrogen interacts with the building units in electrovalent interactions.2 At or below 54 K, the changes of Gibbs free energy indicate that the hydrogen adsorption process is spontaneous. The findings are very encouraging and exciting for synthetic chemists and technologists in terms of the possibility of synthesizing this material as a potential hydrogen storage option in the pursuit of green fuel storage.

Scheme:



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Study of structural, microstructural magnetic and electrochemical properties of $Ni_{0.35}Zn_{0.65}Fe_2O_4$ microspheres

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Abstract:

The structural, microstructural, and magnetic properties along with the electrochemical response of solid microspheres of $Ni_{0.35}Zn_{0.65}Fe_2O_4$ having size ~ 200 nm composed of particles of size ~12 nm, synthesized by template free one-pot solvothermal route have been reported. The results obtained from powder x-ray diffraction, field emission scanning and high-resolution transmission electron microscopic and energy dispersive x-ray spectroscopic techniques suggest that the sample is single phase mixed spinel ferrite crystallized (~ 26 nm) in $Fd\bar{3}m$ space-group with proper stoichiometric. According to dc magnetic study, its blocking temperature is 146 K, the values of its saturation magnetization and coercivity at 300 K and 10 K are 42 emu g−1 and 141 Oe, respectively, and 68 emu g−1 and 290 Oe respectively. The magnetic parameters of the sample are better than its nanometric counterpart [1,2]. The sample exhibits excellent electrochemical performance and can be used as electrode material of supercapacitor battery.

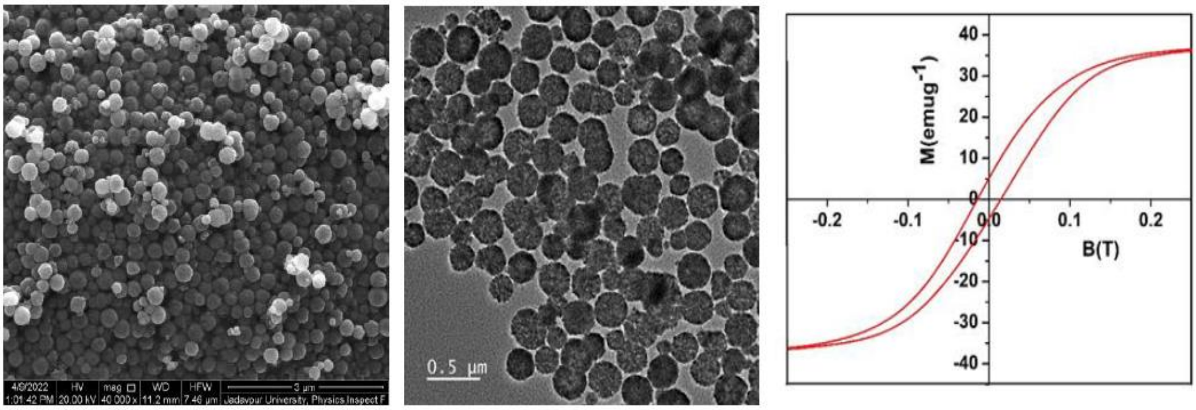

Fig: FESEM image, HRTEM image and MH-loop at 300 K of $Ni_{0.35}Zn_{0.65}Fe_2O_4$ solid microspheres

An ultrafast spectroscopic description of ground and excited state interaction between Cu-doped CdS quantum dots and methyl viologen

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Abstract:

An CdS quantum dots (QDs) are promising materials for optoelectronics, solar cells, metal ion sensing and photocatalysis.[1–2] Doped QDs are especially attractive in this context, due to the disruption of electron-hole correlation in them.[3] This is manifested in the present study, as a more efficient photoinduced electron transfer (PET) to electron acceptors like methyl viologen (MV^{2+}), for Cu(I) doped CdS QDs. Ultrafast transient absorption spectroscopy has been performed, to build a description of the change in excited state dynamics brought about in the process. A careful analysis has been has led to the construction of a Langmuir adsorption isotherm, which unequivocally proves that MV^{2+} ions are adsorbed on the surface of the QDs. Hence, a model involving static as well as dynamic quenching of photoluminescence of the QDs is developed, which addresses the long-standing confusion about unrealistically large values of bimolecular quenching constants, reported often in the literature for systems like these.

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Strategies and challenges in design of fluorescent complexes of a Schiff-base

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Excited state dynamics of neutral and anionic congener of a family of Schiff bases confirms excited state intramolecular proton transfer (ESIPT), segmental motions and hydrogen bond dynamics as major non-radiative pathways in solutions.1,2 Abstracting phenolic protons from the neutral Schiff bases assures enhancement in fluorescence quantum yield and lifetime by taking care of ESIPT.1-3 Chelating Schiff base ligands with a metal ion, especially Aluminium (III) and zinc (II) prevents the conformational motion along with the other nonradiative processes and have shown further improvement in fluorescence responses.1,4 Chelation of the Schiff base ligand with a non-metal boron, belongs to the same group that of aluminium, is expected to show similar order of fluorescence enhancement. In this work, photophysical properties of two organoboron complexes of 2-((2-hydroxybenzylidene)amino)phenol (HBAP) are investigated. Surprisingly, fluorescence quantum yield and lifetime of both the organoboron complexes are very less in non-viscous solvent. Improvement in fluorescence quantum yield and lifetime is achieved in strongly viscous solvent, glycerol. This implies that the effect of chelation is concealed by activation of newer nonradiative channel by a phenyl rotor group, directly attached to boron atom, in less viscous solvent. This contention is fortified by markedly enhanced fluorescence response of the organoboron complexes at cryogenic temperature (77K).

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Theoretical and computational study of metal based superatomic clusters

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Abstract:

Superatomic clusters which exhibits the properties of elemental single atoms are the most important development in the field of cluster chemistry owing to their unique structural and electronic characteristics. It can be used to as building blocks to new materials which may prove to have potential use in the field of optics, sensors, and catalysis etc.

Recent experiences reveal that the determination of atomic structure of the small atomic clusters are difficult in comparison to the characterisation of the bulk material, where techniques like X-ray diffraction and neutron scattering are routinely used. Density functional theory (DFT) plays a vital role in characterising such materials. Evidently, DFT based computations can be proved to be efficient in predicting the structure and physico-chemical properties of small superatomic clusters.

Silicon based clusters have diverse chemical properties and widespread applicability. Bare silicon clusters are not proved to be good building block for materials and doping of these clusters with metal atoms have been shown to introduce stability and make them important candidates for making building blocks of materials having interesting properties. The present work deals with the exohedral heterometal atom doped neutral MSi9M′ systems with M, M′ = Cr, Mn, Fe etc. The relative stability of the clusters has been assessed through DFT.

The structures have been optimized in B3LYP/TZV level of theory and are considered for further investigation. The structure and stability have been explained through molecular orbital and bond orbital analyses. The optimized structures show C2V geometry and represent a stable electronic structure and wavefunction. The analysis of structure and bonding has also been performed with the help of natural bond orbital analysis.

Keywords: Superatomic clusters, Density functional theory (DFT), structure and properties, Silicon clusters, doping, exohedral, transition metal.

Ab initio Potential Energy Surface for astrochemical reaction: CH^+ + O

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Abstract:

The collision between CH^+ with atomic Oxygen is proposed to be one of the crucial sources of CO^+ in the diffused gas cloud of Interstellar medium. In this work, theoretical investigations of the reaction have been carried out using ab-initio quantum chemistry methods. An adiabatic ab-initio Potential Energy Surface (PES) has been reported for the electronic ground state of CHO^+ molecular ion using the multi-reference configuration interaction (MRCI) level of theory with augmented correlation-consistent polarized valence quadruple zeta (aug-cc-pVQZ) basis set. The computed ab-initio data has been fitted to get an analytical representation of the global Potential Energy Surface. The PES fitting procedure of Aguado et. al. was utilized in this work, which has given an elegant fitting of the ab initio data with a root mean square error (RMSE) of 1 kcal/mole. The various reactive pathways on this PES and the presence of various crucial stationary points on the PES were analysed. It is observed that the titled collision happens on $^1A'$ state and leads to two different product asymptotes e.g. {CO^+ + H} and {C^+ + OH}. The exit channel leading to CO^+ is also found to have a small potential barrier at the entrance channel and is highly exothermic in nature. The exothermicity of this channel is found to be ~ 4.02eV.

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Interaction of Lipopeptide with Gram Negative Bacterial and Tumour Membrane

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Abstract:

Research in the continuously increasing threat of polymyxin-resistant multidrug-resistant *P. Aeruginosa* has resulted in development of polymyxin-derived, L-α-γ-diamino butyric acid containing, cyclic lipopeptide FADDI-019 (F19) [1], whose self-uptake mechanism into outer membrane of the bacteria was the focus of this study [2]. Competitive displacement of calcium cations from membrane surface by F19 resulted in increment in bilayer defect size and cooperative insertion of F19 into bilayer interior with barrier height ~1.3 kcal/mol.

Acidic tumour microenvironment (AtμE) acts as a barrier for passive crossing of the cell membrane by chemotherapeutic drugs. Anticancer lipopeptide C6-Pep shows an increased tumour uptake in AtμE [3]. Its accurate protonation state in AtμE was determined using constant pH molecular dynamics [4], which was used to build positively charged fixed protonation approximations of C6-Pep in AtμE and their insertion into tumour bilayer was studied. In AtμE, C6-Pep had lower insertion barrier and destabilizes the bilayer upon insertion.

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Developed Matrix-Free Room Temperature Phosphorescent Carbon Dots for Anti-Counterfeiting Activity

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Abstract:

Nowadays, many researchers are involved in the synthesis of matrix-free room-temperature phosphorescent carbon dots (RTP-CDots) due to their astonishing behaviour. [1,2] Herein, we synthesized matrix-free carbon dots (CDots) through a convenient and facile process. In this regard, Trimellitic acid and ethylenediamine were used as a precursor for the synthesis of RTP-CDots. To establish the mechanism behind room temperature phosphorescent carbon dots, we characterize the synthesized CDots by XPS, HR-TEM, XRD, FT-IR, DLS, FE-SEM, Raman spectroscopy, Zetasizer, UV-Visible, PL, and lifetime decay, etc. The C=O/C=N surface functional groups and hydrogen bonds were responsible for phosphorescence emission, which enable the spin-forbidden transition of S1 to T1 to attain triplet exciton. At 254 excitations, the RTP-CDots have an average lifespan of 287 ms, and a naked-eye observation lasts more than 8 seconds. The RTP-CDots can be used in anti-counterfeiting as it shows dual mode emissions including fluorescence and phosphorescence.

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The role of residues Q1919 and E1920 in G2019S mutated LRRK2 kinase and the searching of these residues for a new homology model, CHK1 kinase

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Abstract

Among more than 40 mutations in Leucine-rich repeat kinase-2 (LRRK2) which are associated with Parkinson’s disease (PD), G2019S mutation in the kinase domain of LRRK2 is the most prominent one [1-2]. The hydrogen bond of residue S2019 in G2019S LRRK2 with Q1919 and E1920 residues were separately reported as the cause of stabilization of the active state of kinase [3-4] so a doubt remained regarding the main responsible residue (Q1919 or E1920) for this process. A mechanistic picture had been presented in our work regarding the stabilization of the active state of kinase using Roco4 kinase as homology model and its relationship with the formation of additional hydrogen bond of S2019 with Q1919 and E1920 which showed both of these bonds were necessary to stabilize the active state of kinase. Also, these residues were searched for the new homology model, CHK1 kinase [5], of LRRK2 kinase domain. Residue K54 and E55 in CHK1 homology were appeared from our investigation as the equivalent residues of Q1919 and E1920 in LRRK2

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Prediction of COMT Inhibitors Using Machine Learning and Molecular Dynamics Methods

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Abstract:

Catechol *O*-methyltransferase (COMT) plays a vital role in deactivating neurotransmitters like dopamine, norepinephrine, etc., by methylating those compounds. The excess deactivation of neurotransmitters can cause Parkinson's disease. However, there are molecules those can inhibit this methylation reaction, termed as COMT inhibitors. Our study is focused on designing these inhibitors by various machine learning methods. First, we have developed a classification model with experimentally available COMT inhibitors, which helped us generate a new data set of small inhibitor-like molecules. Then, to predict the activity of the new molecules, we have applied various regression techniques. Each of the regression models yielded an $R2$ value > 70% for both training and test data sets. Finally, our models are validated with 200 ns classical molecular dynamics (MD) simulations along with an estimation of quantum mechanics/molecular mechanics (QM/MM) method aided methyl transfer energy barrier of the resultant inhibitors.

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Corrosion inhibition performance of synthesized pyrazole derivatives in HCl medium

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Abstract:
Corrosion is one of the challenging problems faced by most industries. So, Corrosion inhibitors are required to overcome the corrosion problem in these industries. Although a large number of organic corrosion inhibitors are reported in the literature most of them are toxic and effective at larger concentrations. Therefore, novel corrosion inhibitors should be effective even at a very lower concentration. Therefore, to find out the mechanism of the action and the inhibitory capacity of 3-((E)-(4-((Z)-(2,3-dimethoxybenzylidene)amino)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-ylidene)amino)benzoic acid (MBAB) against mild steel corrosion in 15% HCl medium and the protection performance of MBAB efficiency is 95.20% at 200 ppm. During adsorption, it was noticed that the MBAB exhibits strong inhibitory efficiency and this phenomenon was discovered to follow the Langmuir adsorption. Furthermore, the thermodynamic parameters were calculated according to the weight loss study. The plots of Potentiodynamic Polarization (PDP) and Electrochemical Impedance Spectroscopy (EIS) demonstrate that the MBAB is a mixed type corrosion inhibitor. FESEM coupled with the (EDX) was used to characterize and analyse the surface of mild steel. Thus, a good correlation between theoretical and experimental results was obtained.

Keywords: *MS, MBAB EIS, FESEM, EDX*

ROS generating Functionalized carbon dots for active Targeted Photodynamic therapy

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Abstract:

Developing therapeutic and imaging functions within a single platform is extremely important to achieve enhanced anticancer efficacy. In this work, N, S co-doped red emissive carbon dots were synthesized from pyromellitic acid, 1,2,4 triaminobenzene dihydrochloride, and thiourea using one pot solvothermal method. The synthesized CDs were characterized by HR-TEM, DLS, XRD, UV-Vis spectrometer, Photoluminescence spectrometer, FT-IR, Zeta Potential, and Raman Microscopy. The obtained CDs have absorbance at 535 nm and show PL excitation independent property with an emission at 605 nm. CDs have an average diameter ranging from 3 to 4 nm. More importantly, these CDs possess the ability to generate singlet oxygen ($^1O_2$) under 532 nm laser irradiation to effectively combat cancer. Further, folic acid was conjugated on the surface of CDs for targeting cancer cells overexpressed with folate receptors. This study highlights the use of CDs as an effective PDT agent for targeted and imaging-guided photodynamic therapy.

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Fabrication of a GUMBOS-based acid-base indicator: smart probe for sensing acids and bases in any solvent.

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Abstract:

The synthesis of a pH-responsive indicator to sense acids or bases in non-polar as well as polar solvents using ionic liquid and anionic dye. Herein, we have assembled a new ionic liquid (IL) comprised of a group of uniform materials based on organic salts (GUMBOS) by attaching a quaternary phosphonium ionic liquid with a very common acid-base indicator, methyl orange, via a simple ion-exchange reaction. This synthesis IL-based indicator is highly soluble in less polar solvents and exhibits good sensitivity toward the presence of acids/bases in those media. Furthermore, this indicator has been used in determining the dissociation constants of several acids in non-aqueous aprotic solvents by overlapping indicator method, and hence this report provides essential information toward the understanding of many fundamental chemical reactions. We further synthesize novel aqueous suspended nanomaterials, i.e., the nanoparticles derived from GUMBOS (nanoGUMBOS) by a simple flash nano-precipitation method. The nanomaterial has been well characterized by different spectroscopic and microscopic(FESEM, AFM) studies (**Fig. A**). The obtained nanoparticles also exhibit substantial pH-responsive behaviors in an aqueous medium and show better susceptibility as compared to the free organic indicator. Thus, this report explores detailed studies on the IL-based indicator in sensing the acidity/basicity of various media (**Fig. B, C**).

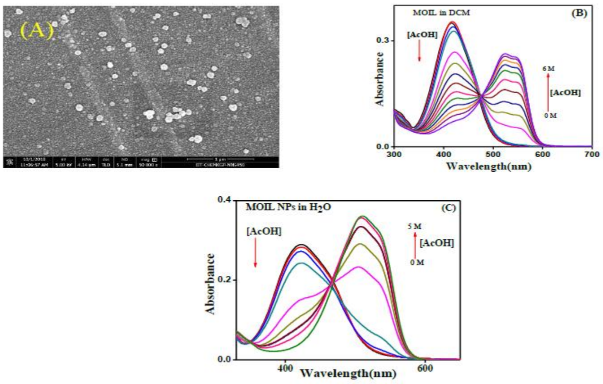

Fig. (A) FESEM image of MOIL nanoparticles, **(B)**. UV-vis absorption spectra of MOIL in the presence of AcOH, (C). Absorption spectra of MOIL NPs as a function of AcOH concentration in water

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Growth of Ga-Doped ZnO Thin Film; Its Electrical and Optical Behaviour

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Abstract:

Ga-doped Zinc oxide (GZO) thin film is an excellent and promising material to be used in organic light-emitting diode (OLED). In this paper, ZnO:Ga transparent conducting oxide (TCO) thin films were deposited on glass substrates by radio frequency (RF) magnetron sputtering techniques. Variations of electrical, optical, and structural properties of GZO films with different substrate temperatures were investigated. Among the different substrate temperatures, 200 °C substrate temperature deposited film shows the lowest resistivity 2.45□10-4 Ω cm with an optical transmission of more than 90%. Finally, GZO thin film was used as an anode material in OLED devices and was also compared with the ITO anode-based OLED. Our GZO based OLED shows similar kinds of performance compared with ITO based OLED devices.

Keywords: Ga-Doped ZnO, Thin Film, OLED

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One pot synthesis of the Lanthanum doped cobalt selenate electrocatalyst towards oxygen evolution reaction (OER) in the alkaline medium.

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Abstract:

There is a continuous demand of traditional fossil fuels, mainly electrical power generation, to transform life in the technical lifestyle. However, the continual burning of limited fossil fuel prompted the urgent need to develop renewable, abundant, and clean energy source. Therefore, for solving the energy crisis, the production of green hydrogen by electrochemical water splitting plays a vital role in achieving this goal. Electrochemical water splitting combines of two half-cell reactions, i.e., Hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). These reactions are kinetically sluggish reactions due to multi-electron transfer reactions. Therefore, the development of an efficient inexpensive catalyst towards HER and OER have been required to accelerate the rate of oxygen and hydrogen evolution. We effectively designed and synthesized sheet-like morphologies of lanthanum doped cobalt selenate through the one-pot hydrothermal route. The successfully synthesized material is first confirmed by carried out different techniques like powder X-ray diffraction (XRD), Field emission scanning electron microscope (FESEM), High-resolution Transmission electron microscope (HRTEM), Selected area electron diffraction (SAED), elemental Energy dispersive X-ray spectroscopy (EDS) and mapping. The as prepared sheet-like lanthanum doped cobalt selenate material is employed as an efficient bi-functional electrocatalyst towards HER and OER in different pH. This electrocatalyst show the low overpotential and the low the Tafel slop value. Also successfully doped with the rare earth metal it show the large exchange current density and the active sites.

Conformational features of receptor binding domain of SARS-CoV-2 in alcohols: A molecular dynamics study

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Abstract:

The concentrated monohydric alcohols have been the most commonly used in alcohol-based hand sanitizers to control transmission of COVID-19. [1] The molecular level of understanding on the interaction of protein and highly concentrated alcohols is essential to understand the deactivation mechanism of the virus. Generally, protein's structural stability and biological function is governed by their dynamic behaviour in the respective solutions. In this work, we performed extensive molecular dynamics simulations and attempts have been made to explore the conformational features and, solvation properties of the receptor binding domain (RBD) of the spike protein in different alcohol solutions. Attention has been given to explore the interactive mechanisms though which the RBD's active residues might be blocked. We observed that RBD exhibits different conformational flexibilities in the different alcohols and in their mixtures which might lead partial unfolding to prohibit its activation. The detailed interactions have been explored and presented. [2]

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A Novel Class of Highly Flexible Transparent Boranil/Polydimethylsiloxane Composites for White Light Emission

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Abstract:

Three triphenylamine-based poly-substituted salicylaldimine (anils) and corresponding N, O-moiety chelated difluoroboron complexes **B1**, **B2**, and **B3** (boranils) have been synthesized and characterized via different spectroscopic techniques. Due to the high luminescence intensity, mechanoluminescent properties, ICT (Intermolecular charge transfer), and significant Stokes shift, boranils have been implemented for light-emitting devices once incorporated inside PDMS (Polydimethylsiloxane), a silicon-based polymer matrix. The **Bm** (a 1:1:1 mixture, w/w, of **B1**, **B2**, and **B3**) covered the more extended emission region in solid and PDMS film and exhibited the white light-emitting tendency. All the individual boranil/PDMS composites showed significant stability when irradiated with UV light and played a crucial role in LED performance. Notably, boranils exhibit white light-emitting efficiency when illuminated on a 325 nm laser with high colour rendering index (CRI) value (96-98 %). They can be enacted in several household lighting applications, including electronic and signalling devices.

This work is recently published as A. Kumari, S. Nandi, and S. Dey, *J. Lumin.*, 2023, **253**, 119466.

Development of in-situ g-C_3N_4 - $BiVO_4$ semiconductor composites for applications in photoelectrochemical Water Splitting

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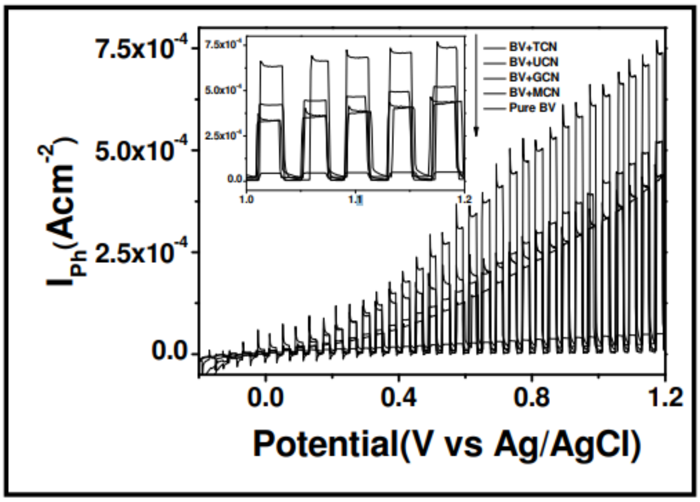
Abstract:

Semiconductor photo electrochemistry (PEC) has received much attention during the last three decades as a promising solution to energy generation and environmental problems. $BiVO_4$ is a promising semiconductor with a moderate bandgap of 2.48 eV for PEC water oxidation. [1, 2] The present report describes the growth of novel in-situ g-C3N4/$BiVO_4$ composites through drop-casting method using $Bi(NO_3)_3$ as precursor salt, melamine, urea and thiourea as the source of g-C_3N_4 followed by annealing in air at 550°C for 3h. Activities of the materials were tested through linear sweep voltammetry and chronoamperometry under chopped illumination for the water oxidation reaction. The optimized thickness of composite bismuth vanadate yields a photocurrent density of ~750 µA/cm^2 using linear sweep voltammetry at ~1.2 V vs. Ag/AgCl, under the illumination of 100mW/cm^2, which is exceptionally higher in magnitude than that of conventionally prepared pure bismuth vanadium oxide particles (45 µA/cm^2).



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Functionalized nona-silicide [Si9R3] Zintl clusters: a new class of super halogens

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Abstract:

In this study,1 using density functional theory, we show that recently synthesized2,3 [Si9{Si(tBu)2H)3}3] and [Si9{Si (TMS)3}3] Zintl clusters not only behave like halogens but also when functionalized with suitable ligands (-CF3, -CN, -NO2) exhibit superhalogen characteristics. Frontier molecular orbitals (FMOs) analyses give insights into the electron-acceptor nature of the Zintl clusters. The potential of these Zintl clusters in the synthesis of new electrolytes in Li-ion batteries is also investigated.

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Green Switching and Light-Harvesting Abilities of Red-Emissive Carbon Nanodot

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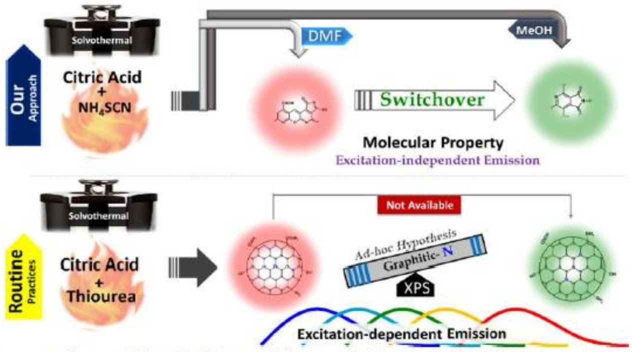
Abstract:

Over a decade in pursuit of photoluminescent carbon quantum dots has created opportunities and left a huge void in understanding the role of graphitic-N in tuning its emission properties. Among the proposed hypotheses on the origin of their emission properties, an emerging one that suggests the formation of molecular crystals lacks the foundations of molecular transformability. Here we observed, solvent reactiveness has been found to manipulate the emission properties of the products derived from a one-pot solvothermal reaction. The excellent superimposition of absorption and excitation spectra and excitation-energy-independent emission of green- and red-emissive products are suggestive of their molecular nature. The best-known graphitic-N in the carbon nanodot turns out to be the nitrogen of citrazinic acid. An unprecedented solvent-directed green switching of the red-emissive product (PR) has been presented here, and the transformed product (PR→G*) shows an uncanny resemblance of spectroscopic properties with the green-emissive product (PG). Being a hybrid photosynthesis system, the chloroplast-red emissive product is found to exhibit a markedly higher rate of reduction of ferricyanide than that of chloroplast alone.



Scheme: Representation of the Solvent-Directed Synthesis of Red and Green-Emissive products with Routine work.

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Improving Stability and Metal-ion Doping of Cesium Lead Halide Nanocrystal: *Tuning Optical Properties for Efficient Photocatalysis*

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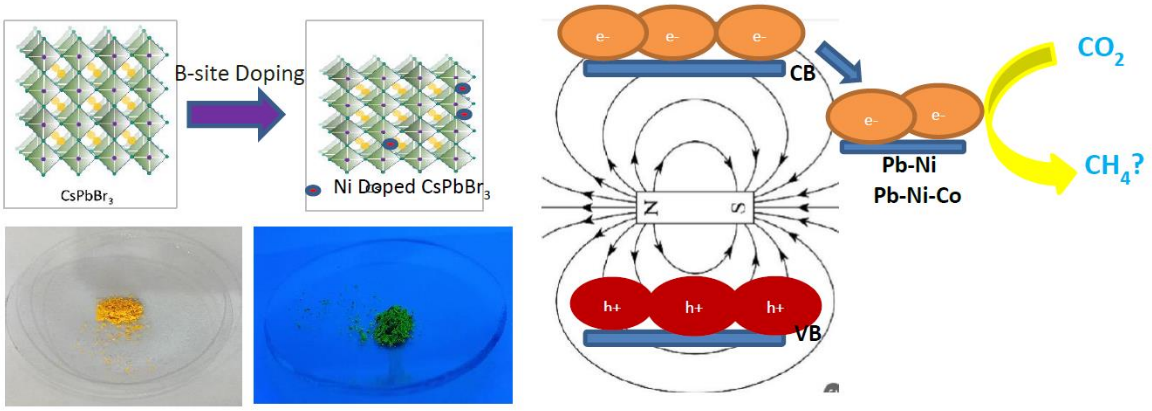
Abstract: Photoluminescent perovskite nanocrystals are mostly used along with base materials such as polymers for material processing and large-scale production purpose. However, the role of polymer in crystal structure engineering and thereby dictating the emission properties of lead halide perovskite nanocrystals is not understood properly. First, we have developed a polymer-directed antisolvent method for synthesis of halide perovskite crystals at room temperature. Surprisingly, hydrophobic polyvinylidene fluoride (PVDF) can reduce the size of perovskite crystals to nano dimensions even at room temperature and increases the stability of the nanocrystal. Afterwards, we tried to increase the stability of the nanocrystal by replacing Lead atom with Ni+2 and perform photocatalysis using it. After doping of ion, the electron hole separation time increased and the dopant is suitable for the photoreduction of CO2 to CH4. Surface passivation was also done using dried Ammonium Thiocyanate. In this work we have introduced magnetic field during the catalysis which will increase the light absorption ability of the photocatalyst.



Scheme: image of the photocatalyst under ambient light and UV light, Graphical representation of the catalytic process.

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Different doped ZnO based TCO film and their different applications

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Abstract:

Transparent conducting oxide (TCO) materials have pay much attention for application in various fields of optoelectronics, TFT and display applications [1-4]. These TCO materials are important components of photovoltaic (PV) devices, OLED because their good electrical and optical properties. Also, their surface properties are much more important for different applications. In order to improve the efficiency of a solar cell, a TCO should possess high optical transmission across a wide spectrum and low resistivity. Furthermore, high transmittance in the visible region and wide band gap of TCOs enhance the electrical performance of PVs. ZnO is of great interest for large-area optoelectronic devices, e.g., flat panel displays, light-emitting diodes, transparent semiconductors, and transparent conductive oxides (TCOs) etc., owing to its good optical properties' transmission more than 90%. In different study Mg, Al, Ga and In doped ZnO thin films are deposited on glass substrate and shows enhanced optical and electrical properties [5]. Electrical, optical, and surface properties are more comparable with commercially established TCO such as ITO, SnO_2 :F. The performance of the ITO TCO degrades under hydrogen atmosphere whereas doped ZnO perform better. In this manuscript authors are reported on different doped ZnO TCO thin film for different application.

Keywords : ZnO, TCO, AFM, XRD, Solar Cell, OLED.

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Physical Chemistry Section Study the Host-Guest Inclusion Complexes of α and β Cyclodextrins with Antidepressant Drugs

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Abstract:

Inclusion complexation of antidepressant drugs with α and β-cyclodextrin were studied systematically. Initially two simple but reliable physicochemical techniques conductance and surface tension were employed to find out saturation concentration for the inclusion complexation and its stoichiometry. The obtained 1:1 stoichiometry was further confirmed by UV-visible spectroscopy and Fourier transform infra-red (FTIR) spectroscopy. Relative stabilities of inclusion complex were established by the association constant obtained from UV-visible measurements, and calculation of conductivity data. Calculations of the thermodynamic parameters dictates thermodynamic feasibility of the inclusion process. The formed inclusion complex was further confirmed by FT-IR spectroscopy. Finally, the cytotoxic activities of the inclusion complexes were analysed and found, non-toxic behaviour of the ICs. This study reveals the formation of inclusion complexes of antidepressants drugs with α and β-cyclodextrin which enrich the drug delivery system without any chemical modification.

Keywords: Antidepressant drugs, cyclodextrin, drug delivery.

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