

CHEMICAL

Warta



Published by

INDIAN CHEMICAL SOCIETY

92, Acharya Prafulla Chandra Road, Kolkata - 700 009, India

Chemical Warta, Vol. : 2, No. : 4, Year : 2021

**January
2022**



Editorial-

Dear colleagues

I wish a prosperous new year to everybody and hope we will be able to overcome the pandemic by the end of 2022. The past two years have been tough, we lost several eminent Fellows and Staff of the Indian Chemical Society, namely, Prof C. L. Khetrapal, Prof S. M. Khopkar, Prof. K. M. Biswas, Prof G. Govil, Prof. Rupendranath Banerjee, Prof. Biswapati Mukherjee, Prof. G. L. Talesara, Prof. Sujit C. Lahiri, Dr. D. S. Bhakuni, and Mr. P.K. Gupta. This has been a severe blow to the Indian chemical Society and the global chemical community in general.

However, even after incurring such heavy losses, we were able to organize virtually the Annual convention of Chemists, ACC-2021 and international conference on Recent Trends in Chemical Sciences, RTCS-2021 on 21-24th December, 2021. Like the previous year, this year too ACC-2021 and RTCS-2021 were organized in different Universities and Institutes virtually. The programme consisted of seven different Scientific Sessions such as Physical Chemistry (CU), Organic and Biochemistry (IISER-Kolkata), Inorganic and Material Chemistry (IIT-Guwahati), Environmental Chemistry (IIT-Ropar), Analytical Chemistry (MS Baroda Univ), Chemical Engineering and Green Technology (ICT-Mumbai) and Industrial and Applied Chemistry (IOCL-Faridabad) Sections.

To encourage the budding young chemists of our country the Society has initiated Young Scientists Conclave organized virtually by the University of Hyderabad in the name of **SSB Young Scientists Award**.

Prof Sridhar R. Gadre (Pune University), Dr. Raksh Vir Jasra (Reliance Industries Ltd, Vadodara) and Prof. Arabinda Das (Burdwan University) received Lifetime Achievement award of 2021. Members of the Council and the Fellows of the Indian Chemical Society were pleased to felicitate them in recognition of their lifetime achievement in the field of chemistry.

Besides Lifetime Achievement Awards there were 16 prestigious endowment awards in the name of 16 Eminent Scientists in the field of Chemistry, which were awarded to Professors and Scientists of different Universities and Institutes across India (13) and USA (3) at the Annual Convention of Indian Chemical Society. The awardees delivered their lectures on their research topics in the field of Chemistry, Chemical Engineering, and related subjects.

A Special Session in the name of Prof. Ashima Chatterjee on her birth centenary year was also organized virtually jointly by School of Environmental Sciences, Jawaharlal Nehru University and the Department of Chemistry, University of Calcutta. Eight invited lectures were delivered by eminent Professors. Their deliberations enriched students and

Chemical Warta; Vol. 2, No. 2; January 2022

Published by: Indian Chemical Society:

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researchers in their respective fields.

Lastly, we would like to thank our honourable President Prof. G. D. Yadav, immediate Past President Prof. D. C. Mukherjee, and all other Council members for their constant support in publishing Chemical Warta. We are also thankful to Dr. Rahul Bhattacharya and other staff members for their help in publishing this online issue of Chemical Warta.

Dr. Nibedita Chakrabarti

Editor



Dr. Gourisankar Roymahapatra Prof. Chittaranjan Sinha

Editor



Editor in Chief





INDIAN CHEMICAL SOCIETY
LIFETIME ACHIEVEMENT AWARDEE, 2021 CONFERRED ON
Professor Shridhar R. Gadre, FNA



Members of the Council and the Fellows of the Indian Chemical Society feel highly honoured to felicitate Professor Shridhar R. Gadre in recognition of his lifetime achievement in teaching and research in the field of Chemistry in general and Theoretical and Computational Quantum Chemistry in particular.

Professor Gadre received his Undergraduate and Master degrees at the University of Pune. He did his PhD with Professor P. T. Narasimhan at the Indian Institute of Technology Kanpur, India. Following his PhD, he did post-doctoral research work with Professor Robert Parr at the University of North Carolina and Robert Matcha at the University of Houston. During his post-doctoral work, Professor Gadre carried out research in density functional theory and on rigorous inequalities in quantum chemistry.

Professor Shridhar Gadre has made significant contributions to theoretical and computational quantum chemistry. These belong to two main research areas: Studies of atomic and molecular scalar fields and the Development of a method for *ab initio* investigations of large molecules and clusters.

His noteworthy research under the first area includes pioneering topological investigations on molecular electron momentum densities and electrostatic potentials (MESP). The latter provides proofs of two basic, general theorems on MESP; definitions of lone pairs and aromaticity as well as the treatment of substituent constants and aromatic sextets via MESP. His works on Shannon entropies in position and momentum spaces for atoms and molecules, leading to a new maximum entropy principle are also widely recognised.

Under the second area, his group formulated a fragmentation-based method called as the Molecular Tailoring Approach (MTA) and a parallel code for implementing it. The method has been applied for geometry optimization and calculation of vibrational IR and Raman spectra of large molecules. His group reported several applications of MTA to large molecules and weakly bound molecular clusters as well as an MTA-based algorithm for a direct and reliable estimation of intramolecular hydrogen bond strengths.

For his contributions, Professor Gadre was elected a fellow of the Indian Academy of Sciences in 1992 and the Indian National Science Academy in 1996 and received the prestigious Shantiswarup Bhatnagar Award in Chemistry (1993).

A dedicated academician, Professor Gadre has contributed significantly to the development of Chemical Education and Research in the country. He has built up a vibrant school of chemists and inspired a large number of students and colleagues who are carrying the torch of his mission.



The Indian Chemical Society sincerely wishes Professor Shridhar R. Gadre a long peaceful life with sound health and continuous academic activities for the advancement and propagation of scientific knowledge.

Professor G. D. Yadav
President
Indian Chemical Society

Professor Chittaranjan Sinha
Honorary Secretary
Indian Chemical Society

Lifetime Achievement Award Lectures

Lifetime Achievement Award Lecture-1 :

Molecular tailoring approach: An art-of-the-possible for ab initio treatment of large molecular systems

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With the advents in computational hardware and software, small-sized molecules became amenable to computation by refined theoretical methods by the turn of the last century. The cost of such high-level calculations, still remained huge, restricting such investigations to medium-sized systems. For treating large molecules by such methods, fragmentation-based approaches have been developed.

This talk will narrate the story of the fragmentation-based quantum chemical calculations from 1970's to 2021. In particular, the molecular tailoring approach (MTA) developed by my research group during the last two decades¹⁻⁵ will be discussed and illustrated with some prototype calculations of energy and vibrational IR/Raman spectra of large molecules and clusters. At the end, I will present the recent application of MTA for efficient construction of a reliable potential energy surface (PES) of a molecule at CCSD(T) level theory.

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INDIAN CHEMICAL SOCIETY
LIFETIME ACHIEVEMENT AWARDEE, 2021 CONFERRED ON
Professor Arabinda Kumar Das



Members of the Council and the Fellows of the Indian Chemical Society feel highly honoured to felicitate Professor Arabinda Kumar Das in recognition of his lifetime achievement in teaching and research in the field of Chemistry in general.

Professor Das received his Undergraduate and Master degrees at the University of Calcutta, Kolkata. He did his PhD at the Jadavpur University, Kolkata. He was a Teaching and Research Associate at the Ohio State University, Visiting Researcher at University of Valencia.

Professor Das has made significant contributions to the metal ion speciation in diverse matrices, correlation of trace metals variation upon low dose radiation on human, low-cost methodology for arsenic and other heavy metals removal from drinking water.

Professor Arabinda Kumar Das was the pioneer in introducing the Environmental Chemistry in 1980 and the Green Chemistry in 2009 at the Postgraduate level of studies. He had rendered stupendous service at the University of Kalyani, West Bengal as the Vice-Chancellor (2004-2009). He has published more than 175 original papers, reviews and invited articles. Professor Das is the author and coauthor of a dozen of higher-level books on Bioinorganic Chemistry and Green Chemistry. He is an activist of People's Science Movement and wrote numerous articles on popular science.

For his contributions, Professor Das was elected Life Member of Indian Chemical Society, Honorary Fellow of West Bengal Academy of Science and Technology.

A dedicated academician, Professor Das has contributed significantly to the development of Chemical Education and Research in the country. He has built up a vibrant school of chemists and inspired a large number of students and colleagues who are carrying the torch of his mission.

The Indian Chemical Society sincerely wishes Professor Arabinda Kumar Das a long peaceful life with sound health and continuous academic activities for the advancement and propagation of scientific knowledge.

Professor. G. D. Yadav
President
Indian Chemical Society

Professor Chittaranjan Sinha
Honorary Secretary
Indian Chemical Society

Lifetime Achievement Award Lecture-2 :

Teaching Green Analytical Chemistry: Methodologies for Green laboratory experiments

Arabinda Kumar Das

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Green Analytical Chemistry (GAC) concepts are not introduced in order to replace the existing ones. New concepts, rather, can be considered complementary to the existing ones and can be studied through the curriculum by giving them the same attention. GAC is also a tool for obtaining information of analytes of different origin, taking into account the safety in the laboratory and with minimal environmental impact, but without sacrificing the analytical requirements viz. sensitivity, selectivity, robustness, accuracy and precision. Recently, good efforts have been made in order to include green chemistry principles to education curriculum, also in the area of analytical chemistry, where twelve principles play the major role. The understanding and awareness of these principles and other evolving related concepts require meticulous teaching of GAC as a part of curriculum at UG and PG levels. This presentation covers the main concepts and challenges of teaching GAC and also adduces the current accomplishment in this field. Teaching GAC must be focused on analytical parameters and practices more than on the incorporation of the so called green parameters to the basic analytical properties. Reduction of risks, energy, reagents and solvents require the search for new innocuous compounds, highest level of information about the samples and measurements and the responsibility of the laboratories about the elimination, and/or reduction and decontamination of the analytical wastes. With this end in view, this presentation comprises a dozen of green laboratory experiments on quantitative analysis in real samples which are based on different aspects of the guiding principles of green and sustainable chemistry, with critical comments; they will be presented as proof of concept of the benefits that could be obtained through greening our teaching practices and will be useful to the students and the teachers of chemistry alike.



INDIAN CHEMICAL SOCIETY
LIFETIME ACHIEVEMENT AWARDEE, 2021 CONFERRED ON
Dr. Raksh Vir Jasra, FNA



Members of the Council and the Fellows of the Indian Chemical Society feel highly honoured to felicitate Dr. Raksh Vir Jasra in recognition of his lifetime achievement in research in the field of Catalysis, Adsorption, Petrochemicals, Nano Porous Materials.

Dr. Jasra has made impactful contributions to Chemical, Defense, Agricultural and Human Resource Development sectors of our country by developing and commercialization of innovative technologies and products.

Dr. Raksh Vir Jasra is presently the Senior Vice President (R&D) of Reliance Industries Limited. Previously, He was the Director Grade Scientist at Central Salt and Marine Chemicals Research Institute, Bhavnagar. He has led R&D groups for the last two decades and developed over 50 and commercialized 16 technologies. He has published 281 research articles, including six chapters in books, and seven review articles in National and International Journals of repute. He has also 64 patents to his name, including 24 U.S. patents with 50 patents in process.

For his contributions, Dr. Jasra has been elected the Fellow of Indian National Science Academy, Indian National Academy of Engineers, Gujarat Science Academy and Life Fellow of Indian Chemical Society. Dr. Jasra is the recipient of many individual and team awards like Prof. S. K. Bhattacharya Eminent Scientist Award by Catalysis Society of India, VASVIK Award, Prof. K. G. Naik Gold Medal by The M. S. University of Baroda, Bronze Medal by CRSI, 5 National Awards from Ministry of Chemicals and Fertilizer, Government of India for innovation in Polymers and Elastomers.

Dedicated academician and professional scientific personnel, Dr. Jasra has contributed significantly to the development of technologies in different sectors like Chemical Sector, Defense Sector, Agricultural Sector of our country. He has built up a vibrant school of professional scientific personnel and inspired a large number of students and colleagues who are carrying the torch of his mission.

The Indian Chemical Society sincerely wishes Dr. Raksh Vir Jasra a long peaceful life with sound health and continuous academic activities for the advancement and propagation of scientific knowledge.

Professor. G. D. Yadav
President
Indian Chemical Society

Professor Chittaranjan Sinha
Honorary Secretary
Indian Chemical Society

Lifetime Achievement Award Lecture-3 :

Developing technologies through innovative chemistry

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Chemistry has been central to providing food, health, material, and mobility security to humankind over the years. This is evidenced by the chemistry led developments in fertilizers and agrochemicals; pharmaceuticals and nutraceuticals; synthetic fibers and polymers and transportation fuels as a response to diverse societal needs. Present challenges of green energy and clean environment faced by humankind provide great opportunity to chemistry researchers to invent and innovate to provide sustainable solutions. Present talk will discuss exciting opportunities arising because of energy transformation from fossil fuels to Hydrogen, Batteries and Fuel cells, Solar and Wind, World is witnessing. Talk will also briefly cover the potential areas needing urgent attention of chemical researchers in the country today. Some of innovative technologies (CPVC technology, 1-Hexene technology, REL-ORCAT process for BTX purification, Novel polymer DPE, New adsorbents for NMP, Sulfolane purification and Sulfur based soil nutrients) developed by us will also be presented in the talk.



Endowment Lectures

Endowment Lecture-1 :

Acharya P. C. Ray Memorial Lecture (2020)

Cholesterol and GPCR function: A molecular sensor for cholesterol in the serotonin_{1A} receptor

Amitabha Chattopadhyay

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G protein-coupled receptors (GPCRs) are the largest class of molecules involved in signal transduction across membranes, and represent major drug targets in all clinical areas. The serotonin_{1A} receptor is an important neurotransmitter receptor of the GPCR superfamily and is implicated in the generation and modulation of various cognitive, behavioral and developmental functions. In our earlier work, we demonstrated that membrane cholesterol is necessary for ligand binding, G-protein coupling and signaling of serotonin_{1A} receptors. In the overall context of high-resolution structures of GPCRs showing bound cholesterol molecules, we previously reported the presence of cholesterol recognition/interaction amino acid consensus (CRAC) motifs in the serotonin_{1A} receptor. In our recent work, we explored the molecular basis of cholesterol sensitivity exhibited by the serotonin_{1A} receptor by generating mutants of key residues in CRAC motifs in transmembrane helices (TM) 2 and 5 of the receptor. Our results show that a lysine residue (K101) in one of the CRAC motifs is crucial for sensing altered membrane cholesterol levels. These observations are further supported from all-atom molecular dynamics simulations which reveal a tightly bound cholesterol molecule between TM1 and TM2 by establishing polar contacts with K101 that leads to stabilization of extracellular loop 1 (ECL1). Interestingly, the position of this cholesterol molecule is almost identical to a co-crystallized cholesterol molecule in the recently reported high-resolution cryo-EM structure of the serotonin_{1A} receptor, thereby strongly validating the molecular mechanism for cholesterol sensitivity of the serotonin_{1A} receptor proposed by us. These results constitute one of the first reports comprehensively demonstrating that cholesterol sensitivity could be knocked out by a single point mutation in a specific cholesterol binding site. We envision that progress in deciphering molecular details of the nature of GPCR-cholesterol interaction would lead to better insight into our overall understanding of GPCR function in health and disease.



Brief Profile: Prof. Amitabha Chattopadhyay is a global leader in membrane and receptor biology and biophysics and is a CSIR Bhatnagar Fellow at the Centre for Cellular and Molecular Biology (CCMB) in Hyderabad, India. In addition, he is a Distinguished Visiting Professor at the Indian Institute of Technology Bombay, Adjunct Professor at the Jawaharlal Nehru University (New Delhi), Tata Institute of Fundamental Research, Indian Institute of Science Education and Research (Kolkata), Swinburne University of Technology (Australia), and Honorary Professor at the Jawaharlal Nehru Centre for Advanced Scientific Research (Bangalore). He served as the first Dean of Biological Sciences at the Academy of Scientific and Innovative Research. Prof. Chattopadhyay received BSc with Honors in Chemistry from St. Xavier's College (Calcutta) and MSc in Chemistry from IIT Kanpur. He obtained his PhD from the State University of New York (SUNY) at Stony Brook, and was a post-doctoral Fellow at the University of California at Davis, prior to joining CCMB.

Prof. Chattopadhyay's work is focused on monitoring organization, dynamics and function of biological membranes in healthy and diseased conditions. His group has developed and applied novel, innovative and sensitive techniques based on fluorescence spectroscopy for monitoring solvent relaxation in membranes, membrane-mimetic media, and proteins. These insightful studies have led to a better understanding of the dynamics of hydration in membranes and proteins. A seminal contribution of Prof. Chattopadhyay's group focuses on the role of membrane cholesterol in regulating the organization, dynamics and function of G protein-coupled receptors (GPCRs), which are important cellular nanomachines that act as drug targets in a majority of human diseases. Pioneering work from his group showed that membrane cholesterol is necessary for the function and organization of GPCRs. In addition, his work has provided novel insight in the role of membrane cholesterol in the entry of pathogens into host cells.

Chemical Warta; Vol. 2, No. 2; January 2022
Published by: Indian Chemical Society:
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Endowment Lecture-2 :

Acharya J. C. Ghosh Memorial Lecture (2020)



emosynthetic livers: Predict, prepare and prove the structure, activity and toxicity of drug metabolites

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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 the subject of 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 scalability¹. We predict structures of metabolites, prepare them on a large scale by oxidation, and elucidate chemical structures². 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 development³.

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Brief Profile: Dr. Mukund Chorghade is a serial entrepreneur and Founder, President and Chief Scientific Officer, THINQ Pharma and Ayurvedya Healthcare Innovations. He is the CSO of APINOVO. He was awarded a DSc by the University of Mumbai in 2021. He provides synthetic chemistry, process and pharmaceutical development expertise to academic laboratories, pharmaceutical and biopharmaceutical companies. His research interests are in Drug Discovery and Development, Process Chemistry Derived Medicinal Chemistry, Traditional Indian and Chinese Medicine. The “Chorghade-Dolphin” sterically protected and electronically activated metalloporphyrin catalysts (“chemosynthetic livers”) find utility in drug metabolism, valorization of biomass and environmental remediation. He is a recipient of three “Scientist of the Year” Awards. He is on the Scientific Advisory Board of corporations/foundations such as APS, Cogent, Empiriko, HSvj, Yew Savin, World Innovation Foundation, Health Sciences Collegium. He is an expert in patent litigation and is a Certified CGLP/cGMP professional.

Chemical Warta; Vol. 2, No. 2; January 2022
Published by: Indian Chemical Society:
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Endowment Lecture-3 :

Professor J. N. Mukherjee Memorial Lecture (2020)

Amphiphilic self assembly in room temperature supercooled solvents

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Self assembly is ubiquitous in nature. Amphiphilic molecules self assemble in water to form dynamic equilibrium structures such as micelles. Micelles are formed by amphiphiles in liquids and undergo random Brownian motion. Recently, we reported formation of dynamically arrested micelles in room temperature supercooled solvents, without using any liquid ingredients. Since all components used in this formulation are solid at room temperature, the supercooled micelles can be considered as a micro- heterogeneous amorphous solid, akin to alloy formation in metals. Small angle X-ray/ neutron scattering provides unequivocal evidence for the formation of micelles in supercooled matrix. The micelles can be formed by dissolving an amphiphile in a mol- ten mixture of sugar (e.g. sucrose, fructose or glucose) and urea or urea derivatives at elevated temperatures ($\sim 70\text{--}90^\circ\text{C}$). These micelles get trapped in a supercooled state upon cooling the mixture to 15°C , forming a sugar glass. This opens a new area of research using room temperature supercooled solvents as the matrix for micelle formation. Unlike normal micelles in water, which form only above the Kraft temperature, these micelles in sugar glass can sustain subzero degree Celsius temperatures (-25°C) without phase separation. The present study shows an example of solid-like assemblies of soft materials, dispersed in another amorphous matrix.

Brief Profile: Dr. P. A. Hassan joined Bhabha Atomic Research Centre (BARC), Mumbai in 1993 and presently serving as Head, Nanotherapeutics and Biosensors Section, Chemistry Division, BARC. He was a visiting researcher at the University of Louis Pasteur, Strasbourg, France in 1995. He pursued his post-doctoral research at the Department of Chemical Engineering, University of Delaware, USA in 2000-2002. He has visited advanced neutron scattering facilities like National Centre for Neutron Research, NIST, Maryland, USA and Institute Laue Langevin, Grenoble, France. He has co-authored more than 160 papers in peer-reviewed journals. His current research interests include microstructure and dynamics of self assembly, polymers, polyelectrolyte-surfactant interactions and nano drug delivery systems. He is an elected fellow of the National Academy of Sciences, India.

Endowment Lecture-4 :

Professor P. K. Bose Memorial Lecture (2020) Walking towards sustainable synthetic methods

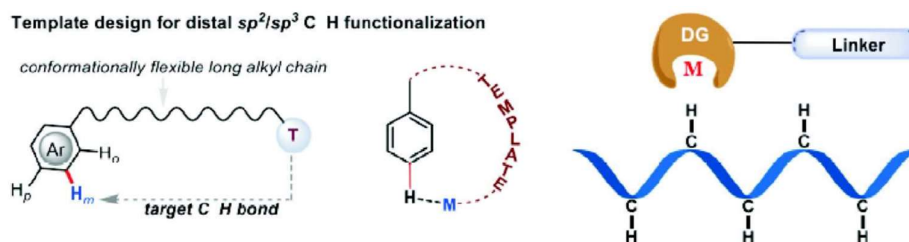
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Mimicking the nature has always been a coveted target for scientific communities. A precise understanding has emerged as to how enzymes accomplish the chemical transformations. Enzymes catalyze inert C-H bond functionalization in a regio- and stereoselective manner using metal-active site. Inspired by the nature, we have developed catalytic methods to functionalize carbon-hydrogen (C-H) bonds which provides significant economic and environmental benefits over traditional synthetic methods. Applicability of our strategies towards synthesis of various complex molecules will be discussed.



Recent References

Science, 2021, **372**, 701; *Nat. Commun.*, 2021, **12**, 1393; *Angew. Chem.Int. Ed.*, 2021, **60**, 14030; *J. Am. Chem. Soc.*, 2020, **142**, 12453; *J. Am. Chem. Soc.*, 2020, **142**, 3762.

Brief Profile: Prof. Debabrata Maiti received his PhD from Johns Hopkins University in 2008 under the supervision of Prof. Kenneth D. Karlin. After postdoctoral studies at MIT with Prof. Stephen L. Buchwald, he joined the Department of Chemistry at IIT Bombay in 2011. His research interests are focused on the development of new and sustainable synthetic and catalytic methodologies. Currently he is an Associate Editor of *Journal of Organic Chemistry*.



Endowment Lecture-5 :

Professor B. N. Ghosh 80th Birthday Commemoration Lecture (2020)

Multifunctional nanocomposites

Jhon Zhanhu Guo

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With the required miniaturization, the materials combining different functionalities have become interesting. In this topic, a variety of advanced polymer nanocomposites will be introduced. Methodologies to prepare nanocomposites and their effects on the produced nanocomposites will be introduced. Unique properties including mechanical, electrical, magnetoresistance etc. and the applications for environmental remediation, energy storage/saving and electronic devices (GMR sensors, strain sensors, electromagnetic interference (EMI) shielding, and electrochromic display windows) will be presented.

Brief Profile: Dr. Guo, currently an Associate Professor in Chemical & Biomolecular Engineering Department of at the University of Tennessee (UT), obtained his Bachelor degree from Shan-dong University of Science and Technology (1996), Master degree from Beijing University of Chemical Technology (1999), and PhD degree from Louisiana State University (2005). All the degrees were from Chemical Engineering. Before joining UT, Dr. Guo was working in Lamar University from 2008-2014 as Assistant/Associate Professor in Dan F. Smith Department of Chemical Engineering. Meanwhile, Dr. Guo had received a three-year (2005-2008) post-doctoral training in the Mechanical and Aerospace Engineering Department at the University of California Los Angeles. Dr. Guo directs the Integrated Composites Laboratory (ICL) and has authored/coauthored more than 800 peer-reviewed journal papers and five issued patents with a total citation of 58,000 and *h*-index of 134. Dr. Guo is the Lifetime Fellow of Indian Chemical Society and the Fellow of the Institute of Materials, Minerals and Mining (U. K.). Dr. Guo's current research team focuses on multifunctional light-weight nanocomposites, especially with polymer and carbon as the hosting matrix to solve the energy and sustainability issues. For more information, please visit <http://composites.utk.edu>.

Endowment Lecture-6 :

Professor Priyadarshan Ray Memorial Lecture (2020)

Anion and ion-pair recognition towards environmental and industrial applications



Pradyut Ghosh

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In general, the presence of certain inorganic anions in excess with respect to their World Health Organization limits in water is a serious risk to millions of people as well as aquatic life worldwide. Inorganic anions like cyanide, carbonate, sulphate, chromate and perrhenate (chemical surrogate of pertechnetate) play significant negative roles towards environmental and water related issues. Moreover, extraction of alkali metal halides has enormous potential applications in separation technology, production of common living materials etc. Thus, encapsulation of anion/ion-pair by artificial receptors is very important, not only due to environmental applications but also for the potential biomedical and industrial applications.

In this century, recognition, sensing and extraction of anion/ion-pair by synthetic hosts have received enormous research attention with promising analytical, industrial and environmental applications. A wide variety of tris(2-aminoethyl)amine, benzene- based, cyanuric acid platform-based receptors containing ammonium, amide, urea groups as anion recognition elements with increasing complexity from tripodal, macrobicycle, molecular capsule to hexapodal have been synthesized by our group

which will be discussed briefly¹. Emphasis will be given on our works which deal with

- (i) trapping cyanide from steel plant wastewater^{2,3}. In steel industries, during the process of production of metal in blast furnace, discharged water contains mostly inorganic pollutants which include complex and free cyanide (linear anion). Thus, the fundamental chemistry of recognition and extraction of cyanide in aqueous medium are considered to be very important to develop technologies in water purification process and industrial waste reprocessing. In this context, as a special case, pilot scale processing of cyanide in steel industrial wastewater will also be presented. (ii) Extraction of alkali metal salts⁴. (iii) Capturing aerial CO₂ as CO₃²⁻ in a molecular capsule and liquid-liquid extraction of SO₄²⁻/CrO₄²⁻⁵. (iv) Extraction of ReO₄⁻ (Fig. 1)⁶.

Chemical Warta; Vol. 2, No. 2; January 2022

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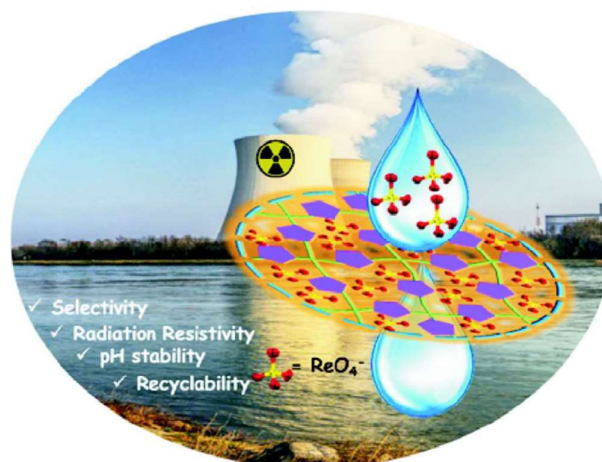


Fig. 1. Removal of ReO_4^- by hexapodal monomeric and polymeric imidazolium receptor (Ref. 5).

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Brief Profile: Prof. Pradyut Ghosh earned his BSc degree and MSc degree from Calcutta University in the year of 1990 and 1992 respectively. Then he did his PhD from Indian Institute of Technology Kanpur under the supervision of Professor Parimal K. Bharadwaj in the year of 1998. Then he joined as a Research Associate in the Texas A&M University, USA under the guidance of Professor Richard M. Crooks. Then he elected as an Alexander von Humboldt Fellow from Kekulé Institute of Organic Chemistry and Biochemistry, University of Bonn, Germany. He joined the Indian Association for the Cultivation of Science, Kolkata, India as an Associate Professor in the year of 2007. Current, he is a School Chairman in the institute. He has achieved several prestigious awards and fellowships in his on-going carrier.



Endowment Lecture-7 :

Professor H. L. Nigam Memorial Lecture (2021)

Biomimetic chemistry-learning from nature to design environmentally benign catalysts

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In nature there are numerous metallo-enzymes which carry out biologically important redox reactions, functionalization of organic molecules, isomerization reactions etc. These reactions are carried out under ambient conditions with high degree of selectivity and specificity. The goal of synthetic chemists is to understand the structure and reactivity of the active sites of these enzymes and to mimic the biological chemistry to produce environmentally benign catalysts of industrial importance. In this lecture few such examples of biomimetic catalysts will be discussed. One such class of enzymes is vanadium dependent haloperoxidases like bromoperoxidase. Several organobromo compounds are known to possess antimicrobial and anticancer properties making them potential candidate for medicinal applications. Several model complexes of vanadium showing bromoperoxidase activity will be discussed in this lecture. We shall also discuss some model complexes of Cu(II) which show ascorbate oxidase and catechol oxidase activities.

Brief Profile: Prof. Chattopadhyay obtained his doctoral degree in Chemistry in 1988 from the Indian Association for the Cultivation of Science. Since the very next year, he is associated with Bengal Engineering College, presently Indian Institute of Engineering Science and Technology. He currently holds a senior professor position at the institute. Prof. Chattopadhyay has worked as a Brain Pool visiting scientist at Advanced Materials Division of Korea Research Institute of Chemical Technology, South Korea from December 2006 to November 2007. He has published 95 papers in International journals. His research focuses on biological and medicinal chemistry.

Chemical Warta; Vol. 2, No. 2; January 2022

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Endowment Lecture-8 :

Professor Dhananjay Nasipuri Memorial Lecture (2020)

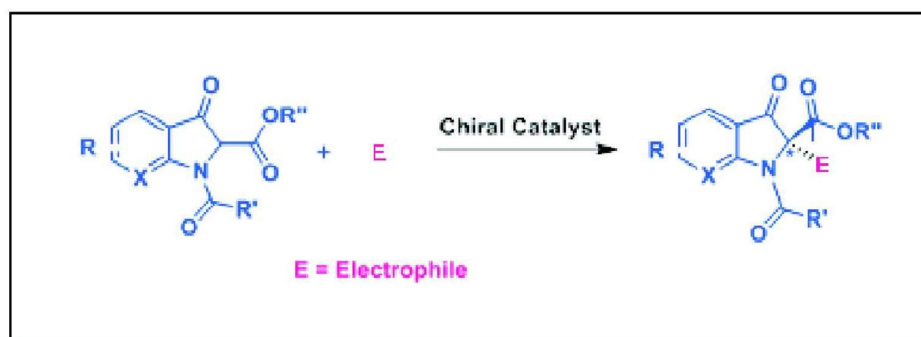
Enantioselective C-N, C-C, C-F and C-S functionalization of 3-oxoindoline-2-carboxylate frameworks

B. V. Subba Reddy

Chief Scientist and Head, Department of Flouro and Agro Chemicals,
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Enantioselective C-N, C-C, C-F and C-S functionalization of 2-substituted-indolin-3-ones has been developed for the synthesis of chiral 3-oxoindoline-2-carboxylate scaffolds using chiral ligands and organo-catalysts. The chiral molecules are obtained in excellent enantiomeric excess and high yields leading to a quaternary stereo center with a broad range of substrate scope.



Scheme

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Brief Profile: Dr. B. V. Subba Reddy is a Chief Scientist and Head of the Department of Flouro and Agro Chemicals, CSIR-Indian Institute of Chemical Technology. He earned his BSc and MSc degree from Sri Venkateswara University, Tirupati (1991) and Sri Krishnadevaraya University, Anantapur (1994) respectively. He did his PhD from Indian Institute of Chemical Technology, Osmania University, Hyderabad (2003) under the guidance of Dr. J. S. Yadav. He did his post-doctoral work from Harvard University (2004-2006), USA (Prof. E. J. Corey, Nobel Laureate) and Max-Planck Institute (2010), Germany (Prof. Herbert Waldmann). His research interests are: Pheromone Application Technology/Semiochemicals, Asymmetric Synthesis (Organocatalysis/ Transition Metal Catalysis), Synthesis of Natural Products/Biologically Active Molecules, etc. He has awarded with several prestigious and both national and international awards and fellowships. He is the life fellow of Indian Chemical Society and several other prestigious organizations. He has published a total of 785 research papers with total no. of citations of 20650.

Endowment Lecture-9 :

Professor D. P. Chakraborty 60th Birth Anniversary Commemoration Lecture (2020)

Properties of $AI_{1-x}B_xPbX_3$ ($A/B = MA, FA, Cs$ and $X = I, Br, Cl$)

D. D. Sarma

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There has been a spectacular rise in the interest in understanding properties of hybrid halide perovskites of the general form $AI_{1-x}B_xPbX_3$ ($A/B = MA, FA, Cs$ and $X = I, Br, Cl$) in view of their spectacular properties, particularly in the context of photovoltaic applications. I shall introduce this subject with some historical background leading to the modern-day excitements to provide a feel for where we stand today before discussing our own efforts to understand physical properties of several of these hybrid materials.

This work is a result of collaborations with B. Bhattacharyya, M. Bokdam, C. De, J. P. Embs, C. Franchini, S. Ghara, T. N. Guru Row, A. Hossain, B. P. Kore, G. Kresse, A. Kumar, J. Lahnsteiner, P. Mahale, A. Mohanty, S. Mukherjee, R. Mukhopadhyay, S. Pal, A. Pandey, M. S. Pavan, S. Picozzi, T. Sander, Sharada G., V. K. Sharma, A. Stroppa, A. Sundaresan, D. Swain and M. Tyagi.

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Brief Profile: D. D. Sarma obtained a 5-year Integrated MSc degree in Physics from the Indian Institute of Technology, Kanpur, in 1977 and a PhD Degree in 1982 from Indian Institute of Science (IISc), Bengaluru. He worked in Kernforschungsanlage (later renamed as Forschungszentrum), Jülich, Germany, as a Visiting Scientist during 1984-1986. He was a faculty member at Solid State and Structural Chemistry Unit of IISc during 1986-2021 and was the first holder of the J. N. Tata Chair of IISc during 2017-2020. He is now serving as an Honorary Professor (2021-2026) and CSIR Bhatnagar Fellow (2021-2024) at IISc. His research interest spans the science of strongly correlated electron systems, primarily based on transition metal compounds, semiconductor nanocrystals and energy materials using a wide range of experimental and theoretical tools. He has published about 500 scientific papers and holds several patents. He is an elected Fellow of all three Indian science academies, the Engineering Academy in India, the World Academy of Sciences (TWAS), and the American Physical Society. He has received many national and international awards and recognitions, including multiple Honoris Causa Doctorate degrees. He has held several academic positions outside of his parent organisation (IISc), including many Honorary/Guest/Visiting Professorships, such as Gaspard Monge Visiting Professor at Ecole Polytechnique (May-July 2019), University Professor of “Computational Material Physics”, University of Vienna (May 2017), Guest Professor of Physics, Uppsala University (2011-2016), Visiting Professor at Department of Complexity Science and Engineering, University of Tokyo (2001-2002), Distinguished Scientist of CSIR (2011-2016), MLS Chair Professor at IACS (2006-2009), Adjunct Professor at TIFR (2003- 2009 and 2011-2014), Honorary Professor at JNCASR (2003-to date) and SNBNCBS (2014-2020), and Distinguished Visiting Professor (2009-2014) and Eminent Visiting Fellow (2018-2023) at IACS. Further details can be found on his group webpage (<https://sscu.iisc.ac.in/people/DDSarma/>) and on his Google Scholar page.

Chemical Warta; Vol. 2, No. 2; January 2022
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Endowment Lecture-10 :

Professor A. S. R. Anjaneyulu 60th Birthday Commemoration Lecture (2020)

Transition metal complexes in stoichiometric and catalytic transformations

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Transition metals, often, bind to appropriate organic moieties to mediate stoichiometric reactions giving rise to the formations of interesting compounds. Although these new compounds, sometimes, have been isolated in the metal bound state. Such stoichiometric transformations become useful for synthetic purposes, if, cheap, easily available reactants and relatively easier synthetic manipulations are utilised. On the other hand, appropriately prepared metal complexes can be used as catalyst for various useful reactions. The presentation would be organized in this background.

Brief Profile: Born in the year 1961 and brought up in the district of Purulia of West Bengal. After completing school from there, got admitted in Jadavpur University in the Department of Chemistry in 1980. After master's degree, joined Indian Association for the Cultivation of Science to step in chemical research. Individual carrier started in the year 1993 after joining North Eastern Hill University, Shillong and after that it has been continuing from Vidyasagar University to the University of Kalyani. Published moderate number of research papers, implemented schemes and a few students have been supervised for PhD degree. Received the fellowship of West Bengal Academy of Science and Technology. Teaching the students of MSc in the areas of Inorganic Chemistry from the very beginning of carrier and have been enjoying the profession.

Endowment Lecture-11 :

Professor R. D. Desai 80th Birthday Commemoration Medal & Prize Lecture (2020)

Chain-folding regulated antibacterial polymeric materials



Suhrit Ghosh

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Despite a rapid growth in cationic host defence peptide (CHDP)-mimicking synthetic antibacterial polymers, the importance of the well-defined secondary structure of the synthetic polymers similar to CHDP has not been studied in context of bacterial membrane perturbation. Recently we have investigated series of cationic amphiphilic alternating polyurethanes (PUs) for antibacterial activity with specific focus on the effect of chain folding on the antibacterial activity. Some of them contain linear flexible hydrocarbons (F-PUs) while others contain cyclic rigid hydrocarbons (R-PUs) in the segmented polymers backbone. F-PUs exhibit intra-chain H-bonding driven pleated structure followed by hierarchical assembly, producing cationic polymersome in water. In sharp contrast, R-PUs, deprived of the chain-folding possibility due to the rigid linker, exhibit immiscibility driven aggregation producing spherical particles. F-PUs exhibit exemplary antibacterial activity with exceptionally low minimum inhibitory concentration (MIC), while R-PUs do not show even moderate activity. Beyond planktonic bacteria, F-PUs also exhibit extraordinary biofilm eradication efficiency. This presentation will focus on the chain-folding regulated self-assembly and antibacterial activity of these newly developed alternating amphiphilic PUs.

Brief Profile: Suhrit Ghosh was born in 1976 in India. After completion of the undergraduate education (Chemistry major) in the Presidency College (now University), Kolkata, he was admitted in the integrated PhD program (Chemical Science) at the Indian Institute of Science, Bangalore in 1997. He received the MS degree (Chemistry) in 2000 and continued for PhD till 2005 under the supervision of Professor S. Ramakrishnan. Then he moved to the group of Professor S. Thayumanavan at the University of Massachusetts, Amherst, USA, for postdoctoral studies (2005-2007). Subsequently he worked as an Alexander von Humboldt postdoctoral fellow (2007-2008) with Professor Frank Würthner at the University of Würzburg, Germany. In 2008 he joined the Indian Association for the Cultivation of Science (IACS), Kolkata, India, as an Assistant Professor where he currently holds the position of a Senior Professor in the School of Applied and Interdisciplinary Sciences and Dean (Academic). He was selected (2009) as an Associate of the Indian Academy of Sciences. He is the recipients of the B. M. Birla Science Prize in Chemistry (2014), Swarna Jayanti Fellowship (2015) from the Department of

Chemical Warta; Vol. 2, No. 2; January 2022

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Science and Technology, Government of India, K. Kishore Memorial Award (2016) from the Society of Polymer Science, India and the Bronze medal (2017) from the Chemical Research Society of India. He has been serving as an Associate Editor for the journal *RSC Advances* since 2015. He is a member of the Editorial Advisory Board of the journal *Macromolecules* since January 2021. Research interest of his group includes supramolecular polymerization of donor-acceptor π -systems, H-bonding driven assembly of amphiphilic π -systems/macromolecules and biologically relevant stimuli responsive aggregation of amphiphilic polymers (poly-disulfides, poly-urethanes). He has published > 110 π papers in reputed international journals. Twelve students have already received PhD from his group.

Endowment Lecture-12 :

Dr. D. S. Bhakuni Award Lecture (2020)

Rongalite: A useful green reagent in organic synthesis

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In this lecture, we would like to describe our work dealing with various applications of rongalite in organic synthesis. For example, we have used rongalite as a useful green reagent for the preparation of benzosultine derivatives, which are the latent precursors to *o*-xylylene intermediates. Several other efforts to expand the utility of rongalite in organic synthesis will also be described. These advances are useful in designing new methodologies for the synthesis of modified amino acid derivatives and peptides and ultimately play important role in drug discovery process.

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Brief Profile: Sambasivarao Kotha graduated with MSc degree in Organic Chemistry from University of Hyderabad and obtained PhD in synthetic organic chemistry from University of Hyderabad in 1985. He continued his re- search at university of Hyderabad as a post-doctoral fellow for one and half year. Later, he moved to UMIST Manchester UK and University of Wisconsin as a research associate. Subsequently he was appointed as a visiting scientist at Cornell University and research chemist at Hoechst Celanese Texas prior to joining IIT Bombay in 1994 as an Assistant Professor. He was promoted to Professor in 2001.

His research interests include organic synthesis, development of new synthetic methods for unusual amino acids, peptide modification, cross-coupling reactions, Metathesis, Chemistry of benzocyclobutene, Green Chemistry and theoretically interesting molecules.

He is a recipient of B. M. Birla Science Prize (1996), N. S. Narasimhan Endowment Award (2000), Bronze Medal, CRSI (2004), IIT-B IRCC Award (2004, 2005, 2010 and 2011) Bhagyatara National Award-Punjab University (2005), S. C. Bhattacharya Research Excellence Award (2008), Prof. Y. T. Thathachari National Award-Bhramara Trust-Mysore (2010), J. C. Bose Fellowship (2010) and CCRS Award (2012). Also, elected Fellow of the Indian Academy of Sciences and National Academy of Sciences India, Indian National Science Academy, Royal Society of Chemistry, Maharashtra Academy of Sciences and Andhra Pradesh Akademi of Sciences. He also served on the Editorial Advisory Board of Indian Journal of Chemistry, Journal of Amino Acids, *Eur. J. Org. Chem.* and *Catalysis Journal*.

Endowment Lecture-13 :

Professor Suresh C. Ameta Award Lecture (2020)

Design and synthesis of efficient TiO₂ based catalysts for visible light induced photocatalytic reaction

Asit Baran Panda

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Owing to one of the most important sustainable energy resources on earth, solar energy harvesting to chemical energy, i.e. development of efficient visible light driven photocatalytic reactions, is getting more and more importance. Till date, plentiful photocatalysts have been developed. However, most of the developed photocatalysts suffer from some serious disadvantages, like limited visible light activity, chemical and

photochemical stability, limited availability and high cost, recombination and so on. TiO₂ is the most studied photocatalyst due to its abundance, low cost, nontoxicity, superior stability and strong oxidizing power. However, it absorbs only UV light due to the wide bandgap, showed phase and facet selective activity, and high recombination rate. Thus needs modification to improve photocatalytic activity and band structure engineering

to make visible light active, through highly crystalline phase and facet selective TiO₂ nanoparticle synthesis, metal or non-metal doping, conducting metal to carbon/graphene impregnation and combination with other semiconductor. We have developed an aqueous peroxo titanium carbonate complex solution as the precursor, a novel precursor for TiO₂ for simple and cost-effective synthesis of nanocrystalline TiO₂. Using the developed precursor, we have synthesized (001) faceted truncated octahedral anatase TiO₂ nanoparticle, nitrogen doped yellow TiO₂ hollow sphere (N-TiO₂), copper impregnated N-TiO₂ (Cu-N-TiO₂), MoS₂ QD decorated TiO₂ nanoparticle. The synthesized (001) faceted TiO₂, N-TiO₂, Cu-N-TiO₂ showed excellent photocatalytic selective organic transformations under 40 W household CFL lamp at room temperature. Whereas the synthesized MoS₂ QD decorated TiO₂ nanoparticle showed excellent visible light induced hydrogen generation activity through water splitting. Catalysts are stable for long run.



Brief Profile: Dr. Panda is a Principal Scientist of the Functional Materials Group of Advanced Materials and Processes Division at the National Metallurgical Laboratory (CSIR-NML), Jamshedpur. He joined here in 2021 after having worked as a scientist for 13 years at CSIR-CSMCRI, Bhavnagar. He obtained his PhD (2004) from IIT Kharagapur and a post-doctoral tenure at BGU Negev Israel, Virginia Commonwealth University, USA and Tohoku University, Japan as JSPS fellow. He has published 122 papers, which have been cited 5541 times and granted 4 patents. His research interest lies in the design and synthesis of size, shape and morphology selective inorganic/graphene/amorphous carbon based nanostructured materials for energy conversion and storage, environmental remediation, heterogeneous catalysis for green chemistry, inorganic pigment and bio-sensor.

Endowment Lecture-14 :

Professor R. S. Varma Memorial Lecture (2021)

Laser spectroscopy: From physics to chemistry, biology and medicine



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Lasers have become an essential light source in spectroscopic applications due to their inherent coherence and intensity. These properties enable both time (fs) and spatial (nm) resolutions required to study materials at the nanoscopic to microscopic level and also their dynamics in femtosecond to seconds time scale. In this talk we will present various applications of laser spectroscopy, particularly vibrational spectroscopy, in physics, biology and medicine.

Understanding molecular movements in the time scales on bond specific vibrational periods have become the focus of recent research with a hope to understanding physical, chemical and biological processes in real time, as in slow motion capture. The third order non-linear susceptibility response of a system using stimulated Raman scattering processes leads to observation of evolution of vibrational structures in femtosecond time scales. We would show examples of energy migration and coherent oscillation of coupled vibrational modes, which provide information on how molecules move and how the environment impacts the dynamics.

In the case of biology and medicine, we would present results of both infrared and Raman microscopic approaches to studying cell-drug interactions, muscle disorders, neuronal stem cell, sepsis and lab-on-chip applications. Further, very recently we have developed a new approach to imaging molecules/chemicals hidden inside containers and masked by other chemicals or tissues. We will present our latest results in this area.



Brief Profile: Siva Umopathy is the current Director of the Indian Institute of Science Education and Research (IISER) Bhopal. He is an Indian laser spectroscopist and was the Chair of the Department of Inorganic and Physical Chemistry and a Professor of Instrumentation and Applied Physics at the Indian Institute of Science. He is known for his studies of molecular dynamics using Raman spectroscopy and is a fellow of the Royal Society of Chemistry and an elected fellow of the Indian Academy of Sciences and also the National Academy of Science of India, The Council of Scientific and Industrial Research, the apex agency of the Government of India for scientific research, awarded him the Shanti Swarup Bhatnagar Prize for Science and Technology, one of the highest Indian science awards, in 2004, for his contributions to chemical sciences.

Umopathy's researches were centered on Laser spectroscopy and he has carried out extensive work on molecular dynamics using Raman spectroscopy. His group also utilizes other spectroscopic techniques like infrared and is involved in the examination of the molecular structure of cells and tissues. Using Raman spectroscopic techniques, he has developed a method to identify biomarkers in cells which is estimated to assist in early cancer detection. He has published several peer-reviewed articles; Research Gate, an online repository of science articles, has listed 164 of them.

Umopathy, holder of Swarna Jayanthi Fellowship (2000) and the J. C. Bose National Fellowship of the Department of Science and Technology from 2010 to 2020, received the Young Investigator Award for the ICORS Conference at the University of South Carolina in 1989 and Sir C. V. Raman Young Scientist Award of the Government of Karnataka in 2003. The Council of Scientific and Industrial Research awarded him the Shanti Swarup Bhatnagar Prize, one of the highest Indian science awards, in 2004. The same year, he received the Bronze Medal of the Chemical Research Society of India. He is also a recipient of the Raman-Mishishuma Award of the India-Japan Science Promotion Council which he received in 2012. He is a fellow of the Royal Society of Chemistry and an elected fellow by the Indian Academy of Sciences in 2003. He has delivered several award orations including the Subbarao Memorial Lecture of Osmania University (1993) and many invited and plenary lectures.

Endowment Lecture-15 :

Professor U. C. Pant Memorial Lecture (2020)

Where there's green, there's growth – Green hydrogen

S. Vasudevan

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Alternative energy sources like solar, wind, thermal, ocean, geothermal, thermonuclear, hydrogen etc., are being considered as possible sources of energy to meet the growing demand. However, none of these energy sources except hydrogen has all the desirable qualities to replace petroleum and natural gas. For example, some are only intermittently available; others are available away from the consumption centers and cannot be used as fuel for transportation. Therefore, out of the above alternative energy sources, green hydrogen is considered the best option, which could form the link between the new energy sources and the user. Hydrogen is the clean and green fuel and when used as a fuel, produces only water. In the hydrogen energy system, it is envisaged that hydrogen will be produced from non-fossil energy sources, and will be used in every applications where fossil fuels are used today. Over the last decade there have been increasing research efforts to investigate the various aspects of the hydrogen energy systems like production, storage and transport and its applications.

Generation of hydrogen via electrolysis is a well-known and established technology. There are two main types of electrolyser [Alkaline and Proton Exchange Membrane (PEM)] and both are well proven and long-lived. Electrolysis has been traditionally based on an alkaline technology, but Proton Exchange Membrane (PEM) electrolysers are now coming to the forefront. However, due to the high cost of both electricity and material, only a small proportion (4–5%) of the worldwide hydrogen production comes from electrolysis. Yet electrolyser costs are expected to drop within the few years as a consequence of standardization, mass-production, and a greater competitiveness. The demand for clean-produced hydrogen and its storage potential spell enormous possibilities for renewable electrolysis in the future. Even non-renewable electrolysis is bound to play an important role in the short-term as a source of moderate amounts of hydrogen for small fuelling stations and domestic applications.

In future low-carbon economics, electrolyser technology could provide a central solution to meeting both the power management needs of the electricity sector and the needs of the transport and industrial sectors for low/zero carbon fuels. Electrolytic hydrogen could thereby displace large proportions of non-electricity fuel consumption. Hence, the new market potential for electrolyser dwarfs the existing market potential and on a global scale it is truly vast.

In this talk some of the important and recent developments in the electrochemical alternatives with newer materials for hydrogen generation are discussed. The talk also covers hydrogen based technologies developed at CSIR-CECRI.

Chemical Warta; Vol. 2, No. 2; January 2022

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Brief Profile: Dr. Vasudevan Subramanian working as Senior Principal Scientist at the CSIR-Central Electrochemical Research Institute and Professor at the Academy of Scientific and Innovative Research, New Delhi. Through my creative, interdisciplinary and cutting edge research, he has made extensive fundamental and applied contributions to the field of water electrolysis, water treatment, inorganic chemicals and storage batteries. His research has focused on novel electro-catalysts, electrolyser anode/cathode, electrochemical water treatment systems, anode/cathode for magnesium reserve batteries and synthesis of inorganic oxidants. Dr. Vasudevan also actively engaged in innovative engineering of PEM based electrolyser, magnesium organic reserve batteries, electrocoagulation and electro-Fenton water treatment systems and electrolysis system for production of inorganic oxidants/chemicals. His assiduous involvement in research on electrochemistry earned DSc (h.c) and ranked in TOP 2% of Scientists Worldwide (Stanford University). Published over 120 scientific papers and two dozen technical patents in his credit and transferred many technologies to industries and has over three decades of research/teaching experience in India's premier R&D institution. He is the Fellow of Royal Society of Chemistry, Australian Institute of High Energetic Materials, Academy of Sciences Chennai and many other academies. He has been nominated as visiting faculty/professor in Indian/International Universities. Prof. Vasudevan is on the editorial boards and associate editor of many prestigious journals including Scientific Reports (Nature) and received numerous professional awards such as MRSI Medal.

Endowment Lecture-16 :

Professor A. K. Chandra Memorial Lecture (2021)

Superatomic chemistry

Puru Jena

Department of Physics, Virginia Commonwealth University,
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Superatoms are atomic clusters with tailored size and composition that mimic the chemistry of atoms in the periodic table¹⁻³. While the chemistry of atoms is governed by the valence electron orbitals, the chemistry of superatoms is governed by their highest occupied molecular orbitals. Because of their specific size, composition, and non-spherical geometry, superatoms not only promote unusual reactions but also serve as the building blocks of a new class of cluster assembled materials with properties very different from conventional materials. This talk will provide the design principles of these superatoms and illustrate their unique role in the chemical and material sciences by focusing on superhalogens that behave like halogen atoms. The electron affinities of the superhalogens, which can be designed and synthesized without using even a single halogen atom, are larger than those of halogens. In addition, unlike atoms, they can be stable when multiply charged and enable noble gas atoms like argon to form chemical bonds at room temperature⁴ and zinc to assume an oxidation state of +3⁵. The talk will also illustrate the role superatoms play in synthesizing water-resistant materials for solar cells⁶, halogen-free electrolytes for solid-state batteries⁷, one-dimensional electrides⁸, and multiferroic materials⁹.

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Brief Profile: Dr. Purusottam (Puru) Jena, Distinguished Professor of Physics at Virginia Commonwealth University received BSc (Hons) and MSc in Physics from Utkal University, India in 1964 and 1966, respectively, and PhD in Physics from the University of California at Riverside in 1970. After postdoctoral and visiting appointments at State University of New York, Albany; Dalhousie University, Halifax, Canada; University of British Columbia, Vancouver, Canada; Northwestern University, Evanston; and Argonne National Laboratory he joined Michigan Technological University, Houghton as an Associate Professor of Physics in 1978. He moved to Virginia Commonwealth University, Richmond in 1980 where he was promoted to Full Professor in 1982. Dr. Jena has remained at VCU ever since with the exception of a year (1986-87) as a Program Director at the Materials Science Division of the National Science Foundation, and a year (2007-08) as a Jefferson Science Fellow and Senior Science Advisor at the US Department of State

Dr. Jena's research covers a wide range of topics in nano-structured materials, condensed matter Physics, and materials Science. These include structure and properties of metals, semiconductors, superconductors, alloys, liquid metals, point and complex defects, surfaces, thin films, atomic clusters, and cluster assembled materials. His current research is focused on three major areas: Structure and properties of nano-clusters and cluster assembled materials (0D), nanotubes and nanowires (1D) and mono- and multi layered materials (2D) with emphasis on energy storage; electronic, magnetic, and optical properties. Dr. Jena is the author of nearly 525 papers including 12 edited books. He has given over 425 invited talks in international conferences and academic institutions in 29 countries around the world and has organized 50 international conferences. He has received over \$12.5 million dollars of funding from federal agencies such as the Department of Energy, Department of Defense, National Science Foundation, and NASA.

Professor Asima Chatterjee Scientific Session

Professor Asima Chatterjee Scientific Session Invited Lecture-1 :

Rosalind Franklin Memorial Award Lecture



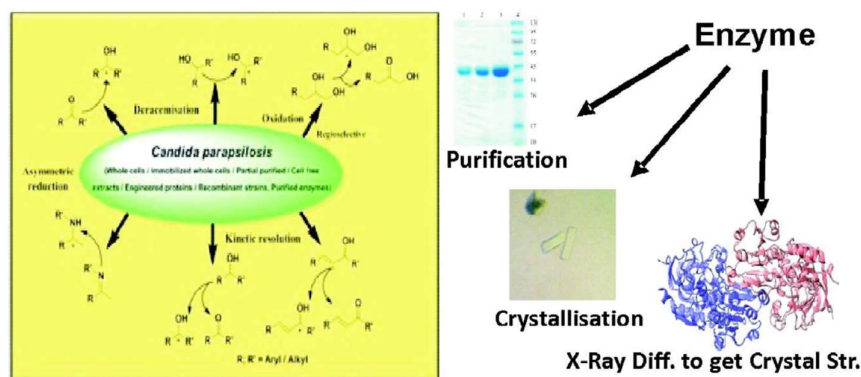
Anju Chadha

Chemistry and Chemical Engineering Department, Indian Institute of Technology Jammu, Jammu-181 221, Jammu & Kashmir

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The uses of biocatalysts, Nature’s environmentally benign catalysts, are rapidly increasing, fueled by an enhanced repertoire of protein engineering tools and an increasing list of solved problems. Enzymes play an increasingly important role as biocatalysts in the synthesis of key intermediates for the pharmaceutical and chemical industry and are an important part of the spectrum of catalysts available for synthetic chemistry. The use of whole microbial cells which are actually micro cell factories which can be effectively employed to generate a variety of organic molecules. We have used the yeast, *Candida parapsilosis* ATCC 7330 over the years to demonstrate its versatility and efficiency in generating a large number of chiral synthons using simple oxidation and re-

duction reactions^{1,2}. The molecular mechanism of the stereochemical preferences of some of these enzymes were studied using purified recombinant enzymes and the native enzymes by X-ray crystallography and biochemical means³⁻⁵. In addition, the lec-





ture will include examples of directed evolution of some important enzymes⁶ which have displaced chemical catalysts and received global attention to minimize environmental damage.

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Brief Profile: Anju Chadha is a Visiting Professor in the Departments of Chemistry, Chemical Engineering and Biological Sciences & Bioengineering at IIT Jammu since September 2021 after retiring from the Department of Biotechnology at IIT Madras as an Institute Chair Professor in June 2020. All through her research and teaching has been in the inter-disciplinary area of Chemical Biology. She did her MSc (Organic Chemistry) from the University of Pune in 1977, taught in Fergusson College, Pune for a year (1978-1979) and then went on for PhD to the Department of Organic Chemistry, Indian Institute of Science Bangalore in 1984. For her postdoctoral work, she was a Fogarty Fellow and then a Visiting Associate (1985-1989) at NIDDK, NIH, Bethesda, USA and a Humboldt Fellow (1992-1993) in the University of Wuppertal in Germany. She was awarded S. K. Chatterjee Award in 2015 given to an IISc alumni and the International Women's Day Award (March 8, 2011) by University of Madras for outstanding contributions to science and technology. Professor Anju is featured as one of the 100 women scientists of India in the book, *Lilavati's daughters*. She worked for six years in a Pharma industry (R & D) before joining IITM as faculty in the Department of Chemistry in 1998. The running theme of her research is Biocatalysis which includes the use of Enzymes in Organic Synthesis and Enzyme mechanisms; Green Chemistry; Biodiesel; Chirotechnology and Biosensors. She has mentored many students - PhD, MSc, MTech, BTech and young school students too. She has published more than hundred and twenty research publications and is a reviewer for projects for the international institutes e.g. in Switzerland and Qatar. She has served on the task force of various committees and Boards at the National level. Professor Anju believes translational research and real life situations which demand science and technological solutions is as important as basic science and has mentored start-ups too. An important issue in scientific research is that of ethics and she was also the first member secretary of the Institutional Ethics Committee at IITM.

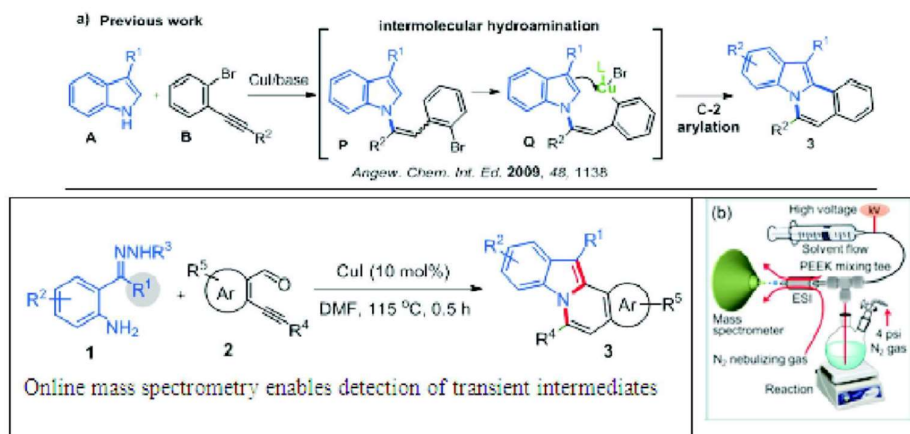
Professor Asima Chatterjee Scientific Session Invited Lecture-2 :

Cu-catalyzed synthesis of indoloisoquinolines via intramolecular hydroamination: Mechanistic insight using online MS

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Hydrazone derivatives have had an enormous impact in the field of synthetic chemistry, because of their potential to undergo valuable transformations¹. In 2009, we have reported the copper-catalyzed tandem synthesis of indolo- and pyrrolo[2,1-*a*]isoquinolines by the preferential nucleophilic addition of N-heterocycles onto *ortho*-haloarylalkynes (intermolecular hydroamination) over N-arylation of aryl halides². In continuation of our ongoing work on the synthesis of N-heterocycles from *ortho*-alkynylaldehydes, we have established a direct synthesis of indolo-isoquinolines by the reaction of amino-hydrazone with *ortho*-alkynylaldehyde via *in situ* generations of in-dole species followed by intramolecular hydroamination³⁻⁶. In this talk, I will discuss our results on the copper-catalyzed synthesis of indolo-isoquinolines and mechanistic identification using the online ESI-MS technique.





References and Notes

IND

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Brief Profile: Prof. Akhilesh K. Verma is presently the Professor, Department of Chemistry, University of Delhi, Delhi. He did his PhD from the University of Delhi in the 2000. The areas of research of Prof. Verma are Superbase-Promoted/catalyzed Organic Transformation, Transition-Metal Catalyzed Organic Transformation, Application of Mass-Spectrometry, and Medicinal Chemistry. He has more than 20 years of teaching and research experience and has guided 32 PhD students and has published 132 research articles of average impact factor 4.3. For his scholastic contribution in research he was elected Fellow of the Indian National Science Academy, Royal Society of Chemistry. He was also awarded with the CRSI Bronze Medal.

Professor Asima Chatterjee Scientific Session Invited Lecture-3 :

Construction of nitrogen containing heterocycles by olefin metathesis

Jyotirmayee Dash

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Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700 032
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Nitrogen-containing heterocyclic systems have received considerable attention due to their widespread science. In this talk, olefin metathesis approaches for the synthesis and applications in pharmaceuticals, agrochemicals, and materials functionalization of nitrogen containing azaspirocycles based on thiazolidinediones, hydantoins and oxindoles will be discussed^{1,2}. The synthesis and functionalization of carbazole ring systems have received considerable attention in organic synthesis due to their widespread occurrence in biologically active compounds¹. New routes for the construction of carbazole ring systems and other indole-fused heterocycles using RCM will be presented. The synthesis of carbazole alkaloids and bioactive indole-fused natural products will be discussed to highlight the importance of RCM. Domino and relay olefin metathesis protocols, for instance, a domino RCM-CM method employing triallyl indole precursors leading to the formation of a new class of dimeric carbazoles will be highlighted².

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Brief Profile: Dr. Jyotirmayee Dash has obtained her PhD degree in Organic Synthesis from Indian Institute of



Technology, Kanpur, India under the supervision of Professor F. A. Khan. She then continued her postdoctoral research first at Freie University, Berlin as an Alexander von Humboldt fellow in the group of Professor H.-U. Reissig, next at ESPCI, Paris with Professor Janine Cossy and subsequently as a Marie Curie fellow at University of Cambridge in the research group of Professor Shankar Balasubramanian. She joined as an Assistant Professor at Indian Institute of Science Education and Research, Kolkata in 2009. She is currently working as a Senior Professor at the Indian Association for the Cultivation of Science-Kolkata.

She has made significant contributions in the structure and function of nucleic acids. Her research interests include new organic transformations, self-assembly of nucleobases and the design and construction of biomolecular devices and artificial ion channels. She has supervised more than 15 PhD scholars and published more than 100 publications in reputed journals (h-index 35, citations 3298). Prof. Dash has been a recipient of DST Swarna Jayanti Fellowship, DBT Wellcome Trust-IA Fellowship, CRSI Bronze Medal and Shanti Swarup Bhatnagar Prize. She has been an editorial advisory board member of ACS Omega (2021), Asian JOC (2021) and Chemical Communications (2020).

Professor Asima Chatterjee Scientific Session Invited Lecture-4 :

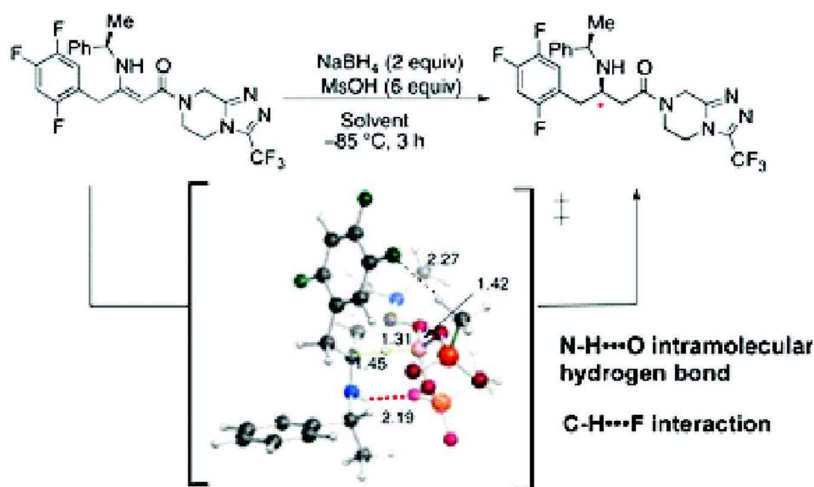
Chemistry at epicentre in Pharmaceutical Industry

Rakeshwar Bandichhor

API-R&D, IPDO, Dr. Reddy's Laboratories Limited, Bachupally, Hyderabad-500 090, Telangana
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As a healthcare requirement to have affordable medicines led to an explosive growth of the branded/generic pharmaceutical industries in recent past. Quite evidently, the pharmaceutical production has come with a significant irreparable environmental damage. As a result, pharmaceutical industry turns out to have higher E-factor. Due to lack of innovative green chemistry, the multi-fold production of active pharmaceutical ingredients (APIs) always concomitantly yields exorbitant amount of waste (E-factor: 25– 120 kg). To get a new drug approved and patented in a competitive pace in a faster manner, quite often, the synthetic route developed turns out to be suboptimal and non-green. Since there is no significant competition to improve patented synthesis before it gets genericized therefore the non-green legacy gets carried forward. Thus, myriad of opportunities arises during innovative research and development of generic APIs towards reducing E-factor and develop cost-effective and green synthetic routes for the





medicines. Most of the pharmaceutical challenges boils down to chemistry understanding and identifying root causes associated with it. Few case studies involving various synthetic strategies to synthesize various APIs e.g. Sitagliptin, Naproxen etc. will be presented.

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Brief Profile: Dr. Rakeshwar Bandichhor is presently Vice President and Head of Chemistry, Process R&D-API, IPDO, Dr. Reddy's Laboratories Limited, Bachupally, Hyderabad. He received his PhD degree from the CSIR- Central Drug Research Institute/University of Lucknow, Lucknow in the year 2001. He did his post doctoral research work in University of Regensburg, Germany, University of Pennsylvania, Philadelphia, USA, and Texas A&M University, USA. Areas of research of Dr. Bandichhor are Asymmetric synthesis, Heterocyclic chemistry, Synthesis of complex molecules, Green chemistry, New methodologies involving organometallic, organocatalytic and biocatalytic approaches. Process chemistry involving AI, PAT and Flow technology for API synthesis. He was awarded with the CRSI Bronze Medal in 2018 and STE Green Excellence Award in 2019. Dr. Rakeshwar Bandichhor has published more than 160 papers in the Journals of international repute and has 25 patents. He has guided 15 PhD students.

Professor Asima Chatterjee Scientific Session Invited Lecture-5 :

Evolution of radioactivity in nuclear medicine – An unending human quest for betterment of

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Mumbai-400 085
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Nuclear Medicine is the branch of medicine which involves the use of radiation in the diagnosis and treatment of diseased states, particularly cancer. Radiopharmaceuticals are radiolabeled molecules designed to target tissues and processes *in vivo* and are used in either diagnostic or therapeutic applications. The design of radiopharmaceuticals involves complex interplay of isotope selection and processing, chemistry and biological studies.

Molecular diagnostic using radiopharmaceuticals is a technique of imaging a diseased state in the molecular level using radiolabeled agents, known as diagnostic radiopharmaceuticals. The radioisotopes used in diagnosis are chemically complexed with a biologically-avid molecule which has target specificity. The gamma photon of the radioisotope used in diagnosis can be of two types, viz. the gamma photon emitters

(^{99m}Tc , ^{111}In , ^{123}I , ^{201}Tl). This photon is used to image the organ in which the radiolabeled molecule localizes using a gamma camera (Single Photon Emission Computed Tomography, SPECT). In case of radioisotopes which emit a positron (^{18}F , ^{68}Ga), the resultant annihilated gamma photon α, β is detected using a Positron Emission Tomography Camera (PET). In certain cases, the diagnostic radiopharmaceutical provides dynamic functioning information of an organ of interest using SPECT or PET. Radiopharmaceuticals designed for therapy in nuclear medicine, are agents which deliver therapeutic doses of particulate and ionizing radiation to the diseased sites. Particulate emission is delivered by radionuclides which decay by emission of $\alpha, \beta, \gamma, \text{Au-}$ Auger- and Conversion-electrons. Recent advances in this area exploit the diversity of receptor-avid and immune-derived molecular vectors as well as a host of therapeutic radionuclides. Therefore, applications of radiopharmaceuticals in nuclear medicine is a multidisciplinary field. An important aspect which governs the success of radiopharmaceuticals is the ability to envisage and thereafter synthesize novel target-specific organic molecules that can chelate radionuclides for diagnostic and therapeutic applications.

This presentation will provide an overview of the evolution of radiopharmaceutical sciences in Nuclear Medicine, with special reference to the relatively recent strategies used for designing of radiopharmaceuticals, for the management of cancer.



Brief Profile: Dr. Sharmila Banerjee is currently the Project Head of the Radiological Research Unit in Advanced Centre for Teaching, Research and Education in Cancer, Tata Memorial Centre. She has been heading the Radiation Medicine Centre and the Medical Cyclotron Facility, BARC, Mumbai. She was the Deputy Chief Executive of Board of Radiation and Isotope Technology (BRIT) and headed all the Regional Centres of BRIT in India. She is a Senior Professor and also a member of the Board of Studies for Chemical Sciences at Homi Bhabha National Institute, Mumbai. She is the Chairperson of the Radiopharmaceutical Committee (regulatory body of DAE). Her current areas of research focus on development of diagnostic and therapeutic radiopharmaceuticals and their clinical translation. The group led by her has achieved the indigenous production of Lutetium-177, in India and demonstration of its use in the preparation of several radiopharmaceuticals for targeted radiotherapy in cancer patients. She has acted as the International Atomic Energy Agency (IAEA) expert on radiopharmaceuticals in several countries under the technical cooperation program. She has been the India-representative in several IAEA-sponsored multi-country coordinated research projects (CRP) and has been designated twice as Chairperson of CRP groups on ^{177}Lu radiopharmaceuticals. She has been awarded the DAE Homi Bhabha Science and Technology Excellence Award in 2010, and also a number of other awards by DAE, Govt. of India. In view of her outstanding contributions in the growth of nuclear medicine, she was awarded the Homi Bhabha Memorial Oration Award of the Society of Nuclear Medicine, India, in 2017. She has more than 250 publications in international journals. She has authored several review articles, book chapters and IAEA technical reports. She is an editorial board member of several international journals. She has also been conferred the prestigious, 'Fellowship Scroll' in 2013, by the Indian College of Nuclear Medicine.

Professor Asima Chatterjee Scientific Session Invited Lecture-6 :

Photoinduced electron transfer reactions: Magnetic field effect

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The mechanism and dynamics regulating photoinduced electron transfer reactions in liquid solutions, rigid matrices and biological systems are the most fundamental problems in photophysical and photochemical primary processes. Along with the studies of electron transfer mechanism in the fluorescence quenching between free donor and acceptor, the identification of the transient species formed in the photo-excited state is necessary for elucidation of the mechanism thoroughly. The laser flash photolysis is one of the most effective techniques in this regard. In addition to that the application of an external magnetic field can affect the electron transfer pathways by alternating the electron spin states of weakly coupled radical ion pairs produced as primary intermediates.

Initially we had focused our work on spectroscopic studies of photoinduced reactions which are quite dependent on the structure of participating molecules and sol-vent. We had used small chemically important molecules to study photophysical and photochemical aspects of inter- and intra-molecular electron/proton transfer, hydrogen abstraction reactions, etc. However, in keeping with current interest in drug-DNA and drug-protein interactions we have extended our studies from small organic molecules to model biomolecules which are therapeutically important and interact with proteins, DNA and photoluminescent chemically engineered carbon nanodots in homogeneous and heterogeneous confined media using steady-state and time-resolved spectroscopy, magnetic field effects and theoretical modeling. Although steady-state and time-resolved studies help to identify steady-state products and transient intermediates respectively, the importance of magnetic field effect lies in its ability to identify initial spin state, one of the deciding factors for ultimate products, as well as to assess the inter-radical distance of geminate spin-correlated radical ion pairs/radical pairs and that is very much useful to study 'distance-dependent' interactions in biomacromolecules. Moreover, the photoinduced electron transfer ability of carbon dots helps to develop their utility as quinone-sensor in live cells.

Chemical Warta; Vol. 2, No. 2; January 2022

Published by: Indian Chemical Society:

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Brief Profile: Samita Basu did her BSc and MSc in Chemistry from Presidency College, Calcutta University and PhD from Jadavpur University in 1989. She did her PhD work on Spectroscopy under the supervision of Professor Mihir Chowdhury at Indian Association for the Cultivation of Science, Jadavpur, Kolkata. After that she joined St. Xavier's College, Kolkata as a Lecturer in Chemistry in 1990. She joined as a Faculty Member at the Chemical Sciences Division of Saha Institute of Nuclear Physics, Kolkata in 1992 and retired from the Institute as a Senior Professor and Head of the Department in December 2018.

The broad area of her research is Spectroscopy focusing on Photochemistry and Spin Chemistry on electron transfer and hydrogen abstraction reactions between small therapeutically important molecules and protein, DNA, nanomaterials, etc. in homogeneous and heterogeneous media. She supervised sixteen PhD students and the number of papers published in peer reviewed journals including book chapters is more than one hundred and fifty. Along with her research work she used to teach MSc students at Calcutta University and Bidhannagar College. She was elected as a Fellow of the West Bengal Academy of Science and Technology in the year 2010 for her contributions in the field of Molecular Spectroscopy. She was awarded Professor P. K. Bose Memorial Award, Indian Chemical Society in 2012. She was also an Executive Committee member of International Spin Chemistry for fifteen years. She was superannuated from Saha Institute of Nuclear Physics in December 2018. However, she is continuing her research work and also teaching at Calcutta University, Bidhannagar College, Barasat University and JBNSTS, Kolkata as a guest teacher.

Professor Asima Chatterjee Scientific Session Invited Lecture-7 :

Scalable ultrathin CdS/CdTe photovoltaic device

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Chemical Bath Deposition process is developed to deposit ultrathin low cost solar cells. Semi-transparent CdS-CdTe photovoltaic cells of less than 600 nm thick are fabricated. By controlling the thickness of the films, the devices can be made semi-transparent and can be used as window panes and skylights in buildings. These photovoltaic cells, being p-n junction based inorganic cells, are stable under varying atmospheric conditions. Thus, in addition to weather control, these window panes and skylights can act as energy harvesting systems.

Brief Profile: Dr. Sheela K. Ramasesha completed her BSc and MSc from Bangalore University, before joining the Indian Institute of Science (IISc) for pursuing PhD under the guidance of Professor C. N. R. Rao and worked on the electrical and magnetic properties of low dimensional materials. Subsequently, she was a post-doctoral fellow in Oxford University, UK and Princeton University, USA. After returning to India she briefly worked in IISc before joining the National Aerospace Laboratories (NAL). At NAL she carried out high pressure studies of electrical and structural transformations in solids. She successfully initiated work on high-pressure high-temperature synthesis of molybdenum disilicide for high temperature applications through a DST project. In 2001, she joined GE-GRC as a materials scientist and later managed the ceramic synthesis lab which she helped in founding. During her stay in GE, she worked on interconnects for solid oxide fuel cells and on renewable energies, resulting in many patents and internal publications.

Recognizing the importance of alternate energies for the future, Dr. Sheela began her pursuit of research in that field at IISc. She has worked on identifying suitable solar technologies/ for tropical conditions and has successfully planned, designed and installed a 20 kWp solar roof-top photovoltaic system in IISc. She carried out studies on solar power generation from roof-tops of fast moving train coaches. The Railway Ministry has taken this up for implementation. She has carried out pilot experiments in a remote weaver's village on employing stored solar energy to enhance productivity and enable children to study at nights. She has given talks in many workshops on popularising renewable energy technologies.

Dr. Sheela has modelled diffusion of particulate matter from emissions of coal-fired thermal plants. This study will quantitatively correlate increase in incidence of respiratory diseases with increased emissions. She has also emphasized on adopting solar thermal technologies in India.

Dr. Sheela has published over 100 papers in peer reviewed International Scientific Journals in addition to writing many popular articles on issues like pollution and water usage. She also holds 6 international patents. She has also authored a frictional novel "The Meticulous Plan".

Chemical Warta; Vol. 2, No. 2; January 2022
Published by: Indian Chemical Society:
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Professor Asima Chatterjee Scientific Session Invited Lecture-8 :

A Tribute to My Teacher Professor (Mrs) Asima Chatterjee

Bani Talapatra

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Professor (Mrs) Asima Chatterjee is an iconic personality in the Indian Science scenario. Her name commands admiration, honour, and reverence. Her contribution on the Chemistry of Plant Natural Products is enormous. She obtained the DSc degree of the Calcutta University in 1944. Incidentally, she was *the First Woman to obtain the DSc degree of any Indian University*. She received many distinctions in her scintillating career – mention may be made of a few prominent ones: *Fellow of the Indian National Science Academy (FNA)*(1960), *Fellow of the other major Science Academies of India*, *Santiswarup Bhatnagar Award* (1961), *General President of the Indian Science Congress Association (ISCA)*(1975), “*Padma Bhushan*” by the Govt. of India (1975), *Sir C. V. Raman Award* (1982), *A Member of Rajya Sabha* (February 1982–May 1990) – *all crowning attainments*, in addition to a string of *prestigious Awards*. In this talk I will attempt to state, among other matters, some of my personal interactions with her.

Brief Profile: Bani Talapatra taught natural products chemistry at Calcutta University (CU) for more than three decades, in some other universities of West Bengal and Tripura as a Guest Teacher for more than a decade, and lectured in many universities as a resource person of the UGC Refresher Courses. She taught general chemistry in Victoria Institution (College) for several years during her early career.

She obtained the DSc degree (2nd lady of CU) working under Professor (Mrs) Asima Chatterjee and then joined a Postdoctoral Fellowship at the Microbiology Department, Vanderbilt University (VU) with the renowned microbiologist, Professor V. Najjar. At VU she learnt much about organic reaction mechanisms from Sir C. K. Ingold (Visiting Professor) for few months.

After more than 3 years of her return she joined the Chemistry Department of the CU as Lecturer and eventually became Professor and Head of the Department. As a UNESCO Senior Visiting Scientist (in 1976 and 1983) she was briefly associated with about 2 dozens of outstanding scientists, Professors of major universities of USA, UK, Germany, and Japan. She also participated in more than 25 International Conferences in USA, Europe, S-E Asia and India.

Her research interests include various aspects of natural products chemistry including terpenoids, alkaloids, polyphenolics, reaction mechanisms and stereochemistry. She published more than 130 research papers and 15 students obtained a PhD degree of the CU under her guidance. She mentored more than 50 PhD and post-doctoral students during their research.



She co-authored with her husband Professor Sunil Kumar Talapatra a unique text-cum-reference Book titled “**Chemistry of Plant Natural Products: Stereochemistry, Conformation, Synthesis, Biology, and Medicine**”, with a Foreword by Professor K. C. Nicolaou, published by Springer-Verlag, Berlin, Heidelberg (March 2015, 2 Vols, total pages 1280+LXIII), which will remain a classic in the field.

She acted as the Organizing Secretary of the “*National Symposium on Contributions of Women in Science (2018)*”, under the aegis of ISNA, **first of its kind in India**, with Professor Sunil Kr. Talapatra as the President.

She served **The Indian Chemical Society as *The Scientist-in-Charge of the Organic Section*** for 3 years during its *3 Annual Conventions* and as a Council Member.

She is a co-author with Professor S. K. Talapatra of a monograph titled “**Basic Concepts in Organic Stereochemistry**”, with a Foreword by Professor Goverdhan Mehta, FRS, to be published by Springer-Nature, London in early 2022, now in print.

She is a Life Member of (i) the Indian Science Congress Association, (ii) the Chemical Research Society of India, Bangalore, (iii) the Indian Science News Association, (iv) the Indian Chemical Society and (v) the Indian Association for the Cultivation of Science.

She wrote a book titled “*More Anubhabe*” containing a collection of Bengali poems (2nd edition, 2001), and another book titled “*Aami Hridayer Kathaa Bolitey Byaakul*” containing a collection of Bengali and English poems and Bengali articles (2nd edition, 2016).

Young Scientist Conclave

Young Scientist Conclave Invited Lecture-1 :

Transition metal complexes of *N*-heterocyclic carbene ligands: Impact of the ancillary ligands in their catalytic activities

Arnab Rit

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Chennai-600 036

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Ancillary ligands are known to play crucial roles in the catalytic activity of any metal complexes and their stereoelectronic parameters are normally considered as important factors to tweak their properties including catalytic activity. Over the past few decades, *N*-Heterocyclic carbenes (NHCs) have established themselves as an important class of ligands in various fields including homogeneous catalysis¹. Although extensively utilized in catalysis, detailed study on the combined steric and electronic influence of the ancillary NHC ligand in transition metal catalyzed various (de) hydrogenation processes are rather limited². Detailed understanding of this type would definitely provide useful input for future catalyst developments. To study such effects, we have synthesized a series of Ru^{II}-complexes with either orthometalated CNHC Cphenyl-bidentate NHC ligands or unsymmetrical chelating ligands where an imidazolylidene (ImNHC) is coupled to a pendant triazolylidene (tzNHC)/N-donor (Fig. 1). To understand the influ-

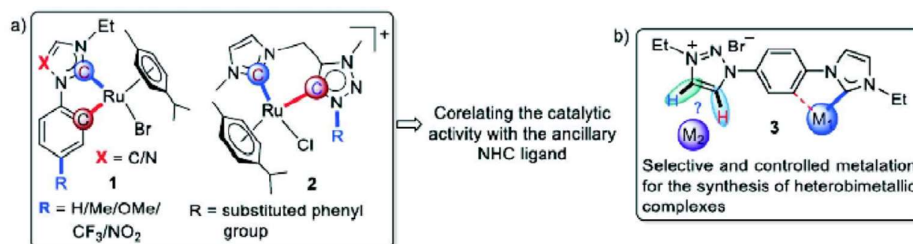


Fig. 1. (a) Ru^{II}-NHC complexes used in this study and (b) ligand design for the synthesis of heterobimetallic complexes.

ence of such ligand variations, all these complexes were applied in hydrogenation as well as borrowing hydrogen (BH) reactions which revealed that substantial tailoring of catalytic activity is possible by altering their steric and electronic profiles³. Further, the change of the bridging unit from CH₂ to phenyl group allows access to diverse heterobimetallic complexes, via selective and controlled metalation, for application in tandem catalytic transformations.

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

Young Scientist Conclave Invited Lecture-2 :

A nickel catalysed alcohol oxidation and N-alkylations mediated by hydrogen atom transfer

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The N-alkylation of primary amines to higher amines is of importance for the synthesis of various biologically active molecules. Previous reports for the synthesis of secondary and tertiary amines via alkylation of primary amines involve toxic chemicals and harsh reaction conditions. In the present work, we attempt to explore environmentally

benign synthesis of higher amines employing inexpensive and readily available alcohols as alkylating agents, generating water as the only by-product¹. The redox non innocent ligand backbone in the catalyst plays an important role to do efficient conversion. Indeed, it has been observed that a hydrogen atom transfer (HAT) is the crucial step to further alcohol oxidation, which is in stark contrast to traditional M-L bifunctional activation of a bond. Detailed kinetic studies and isotope effects elucidate the mechanistic sketch further which helps us to extend the scope of the reaction in broader field.

Understanding the dehydrogenation process helped us further to fabricate a series of heterocycles and study the dehydrogenation of N-heterocycles²⁻⁷.

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

Chemical Warta; Vol. 2, No. 2; January 2022
Published by: Indian Chemical Society:
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Young Scientist Conclave Invited Lecture-3 :

Manipulating molecular and material properties by strong light-matter coupling

Jino George

Indian Institute of Science Education and Research Mohali, Mohali-140 306, Punjab



Strong light-matter coupling is an emerging interdisciplinary area of research. Here, I will introduce a new form of matter called polaritonic states (half-photon - half-matter states). We recently found that strong coupling can control both the chemical and physical properties of matter by generating polaritonic states. In this talk, I will be focus- sing on chemical reaction control - a.k.a. polariton chemistry -, a recent development from our lab at IISER Mohali. The later part of the talk will be on the coherent behavior of the polaritonic states in the energy/electron transport process in the coupled system. The talk will conclude by discussing the future perspectives of this emerging area.

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4. J. Lather, P. Bhatt, A. Thomas, T. W. Ebbesen and J. George, *Angew. Chem. Int. Ed.*, 2019, **58**, 10635.

Brief Profile: Dr. Jino George is an experimental physical chemist by training. He received his PhD on chiral plasmonics (2012) from CSIR-NIIST Thiruvananthapuram. Later, he spent five years at the University of Strasbourg, France as a post-doctoral fellow. At Strasbourg, he studied the effect of strong light-matter interaction on the chemical and physical properties of coupled molecules and materials. At IISER Mohali, his studies are focused on understanding the properties of hybrid light-matter states and its application in controlling chemical reaction rates. He is also interested in studying the transport behavior of electromagnetically dressed 2D materials.

Young Scientist Conclave Invited Lecture-4 :

Synthesis and biological investigation of natural products and designed molecules

Kiran Kumar Pulukuri

Department of Chemistry,

Indian Institute of Science Education and Research Tirupati, Tirupati-517 507, Andhra Pradesh



Natural product's (NP's) produced by living organisms have long been a source in the discovery of new drugs to treat life threatening diseases. In addition to their role in drug development, NP's have produced profound impact on the field of chemical biology, in identifying important new cellular functions and signalling pathways. The chemical synthesis of NP's with unique structural and biological properties remains a daunting challenge to the synthetic chemists. Research in the field of NP synthesis has changed from focusing only on the synthesis of a specific molecule to the development of strategies that enable the structural modification's and synthesis of a broad family of natural products. In recent years NP's synthesis became even more challenging due to the new environmental regulation and increased production costs, which increased the demand to develop new greener and cost-effective strategies. Synthetic organic chemists are well poised to meet these challenges and complexities associated in natural product-based drug discovery by adopting new technologies such as flow chemistry, bio-catalysis, C-H functionalization and redox processes. For the past few decades, a number of robust and scalable strategies for natural product's and their derivatives were developed through a semi synthesis or total synthesis, which resulted in the successful development of many drugs.

Synthesis and biological evaluation of natural products prostaglandin J₃, CJ-16,264 and tubulysin and their derivatives will be presented. Also, a novel strategy to synthesise the eudesmane family of natural products will be discussed.

Brief Profile: Dr. Kiran Kumar Pulukuri is an Assistant Professor in the Chemistry Department at the Indian Institute of Science Education and Research, Tirupati, India. Dr. Kiran received a BSc degree in physical sciences from the Osmania University, India, in 2005 and a master's degree in Chemical Sciences from Pondicherry University, India, in 2007. Later, he joined Prof. Tushar K. Chakraborty's group at IICT, Hyderabad, India, for PhD and graduated from JNU, Delhi, India, in 2013. After post-doctoral work with Prof. K. C. Nicolaou at Rice University (2013-2019), Kiran returned to India to start his independent research group in 2019. His contribution to the field of organic synthesis is reflected from his 19 publications in highly reputed international journals and 5 US patents. Dr. Pulukuri, is a recipient of Eli-Lilly Asia Outstanding Best Thesis Award (year 2013) and Elsevier outstanding reviewer award (year 2017). His research interests are focused on the synthesis of biologically active natural products, asymmetric catalysis, and drug discovery.

Chemical Warta; Vol. 2, No. 2; January 2022

Published by: Indian Chemical Society:

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Young Scientist Conclave Invited Lecture-5 :

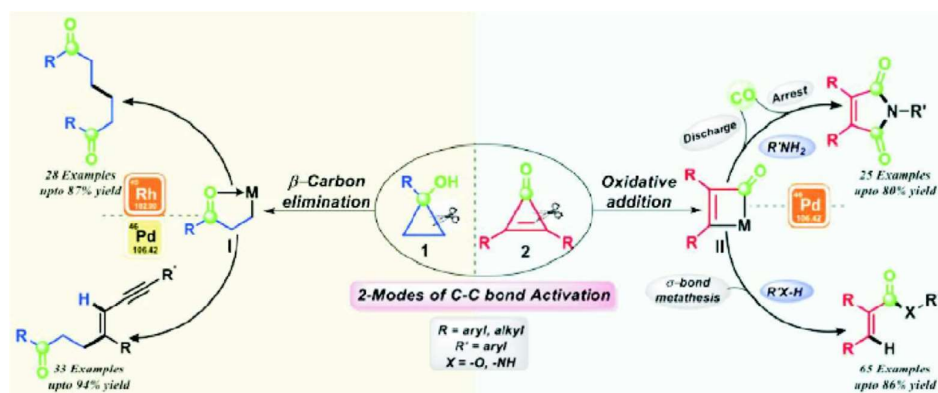
Strained organic molecules as 3C synthons: C-C Bond activation as a tool for the synthesis of N-heterocycles and privileged structures



Ponneri C. Ravikumar

National Institute of Science Education and Research (NISER) Bhubaneswar, Bhubaneswar-752 050, Odisha

Transition metal-catalyzed C-C bond activation is currently a developing area, it has dramatically expanded chemist's toolbox for the synthesis of complex organic scaffolds. Numerous synthetic protocols have been demonstrated by taking advantage of the inherent strain of 3-membered cyclic system.



In this regard, cyclopropanol **1** and cyclopropanone **2** chemistry is still elusive. We have developed new catalytic system that proceed mainly via β -carbon elimination and oxidative addition of C-C bond to the transition metal. In one case, we have generated homoenolate **I** from cyclopropanol **1**, which undergoes functionalization to generate diverse β -functionalized scaffolds. Here, we report a rhodium¹ and palladium² catalysed C-C activation of cyclopropanol to generate diverse 1,6-diketone and 1,3-enyne molecules respectively.

On contrary, cyclopropanone **2** in the presence of palladium catalyst leads to four membered palladacyclobutenone **II**. The intermediate **II** can discharge and arrest one

molecule of carbon monoxide to generate palladacyclopentendione, that has been further functionalized in presence of structurally diverse anilines to deliver maleimide derivatives with the release of hydrogen gas (detected in GC)³. In another case, palladacyclobutane **II** underwent α -bond metathesis in presence of phenols and anilines to give α -unsaturated esters and amides⁴.

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Brief Profile: Dr. Ponneri C. Ravikumar obtained his BSc (Chemistry) and MSc (Organic Chemistry) from the University of Madras. He completed PhD at the Indian Institute of Science, Bangalore, India, under the guidance of Professor A. Srikrishna. He completed post-doctoral research with Fraser Fleming at Duquesne University, PA, and with Professor Seth B. Herzon at Yale University, CT. He joined as Assistant Professor position at the Indian Institute of Technology, Mandi, India. He continued there till December 2015, then he moved to National Institute of Science Education and Research Bhubaneswar, where he is currently an Associate Professor.

Young Scientist Conclave Invited Lecture-6 :

In situ synthesis and cyclisations of ambiphilic allenes

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Allenes are important reactive intermediates and building blocks of many important natural and synthetic molecules^{1,2}. Our group at University of Hyderabad is engaged in tuning the ambiphilic reactivity of allenes through the regioselective approach to accomplish the synthesis of privileged molecules particularly through annulation reactions³. In most cases, we perform a S_N2 reaction with propargyl alcohols and suitable nucleophiles to get *in situ* generated tetra-substituted allenes under Calcium catalysis. Annulation proceeds through an intra-nucleophilic attack (attached to allene) and follows a cascade process to deliver the designed compounds.

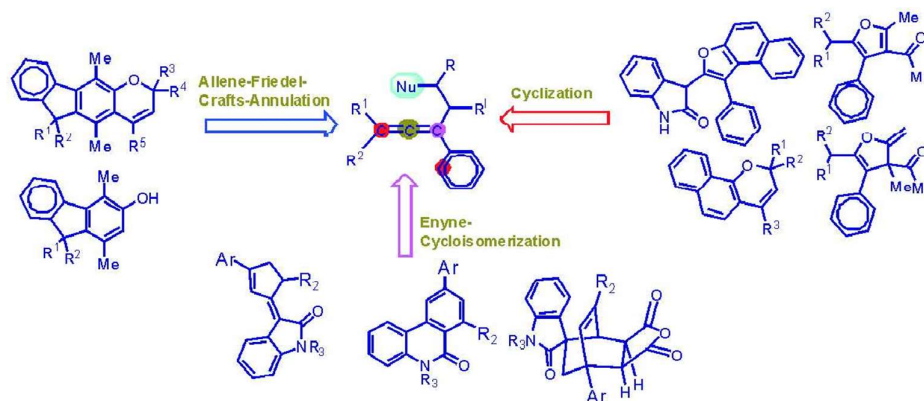


Fig. 1.

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Brief Profile: Dr. Srinivasarao Yaragorla obtained his PhD in Synthetic Organic Chemistry from ICT-Hyderabad in 2008. Subsequently, he did a couple of post-doctoral stints at the University of Minnesota, USA and the University of Hyderabad (2008-2012). Then he joined the Central University of Rajasthan as Assistant Professor in 2012. Later, he moved to the University of Hyderabad and currently, he is Associate Professor in the same place.

His research group engaged in the development of new synthetic strategies that commence from simple, readily available or easily preparable chemicals under sustainable catalytic conditions. The broad areas include, (i) *in situ* synthesis of allenes and their cyclization reactions; (ii) harnessing the ambiphilic reactivity of *in situ* formed C-acylimines to construct important heterocycles flexibly and straightforwardly; (iii) C-H functionalization reactions; (iv) enyne-cycloisomerization reactions. The group successfully demonstrates the calcium salts as an alternative, sustainable Lewis acid catalysts for many of the organic transformations. He has authored more than 65 publications, having a thousand citations with 19 *h*-index. Under his mentorship, four PhD's were awarded, and currently, six students are pursuing their PhD. He has delivered several invited lectures in reputed national and international conferences, Academic Staff Colleges (HRD Centres), and Science academy refresher Courses.

He was a recipient of D. S. Kothari post-doctoral award from UGC; Fast Track Young scientist, and Travel grant awards from DST. He was selected for the Associateship of the Indian Academy of Sciences (IASc). He also received Prof. S. Jaya Ramireddy excellence award from S. V. University, Tirupati.



Young Scientist Conclave Invited Lecture-7 :

Dimensionality reduction in coupled cluster theory: Machine learning and analytical approaches

Rahul Maitra

Indian Institute of Technology Bombay, Mumbai-400 076



Coupled cluster theory, owing to the exponential parametrization of the waveoperator, is highly nonlinear and often solved iteratively. However, due to high computational scaling of the amplitude determining equations, its application is limited to small to medium sized systems. In this talk, I will analyze the associated iterative scheme as a multivariate time-discrete map from the perspective of nonlinear dynamics. I will demonstrate that the iteration dynamics is dictated by a small subgroup of ‘master’ amplitudes, mostly involving chemically active orbitals, while all other amplitudes are enslaved. Starting from a few training iteration steps to establish an inter-relationship among the variables, we employ various supervised machine learning models to dynamically express the enslaved amplitudes as unique functions of the master amplitudes. This leads to tremendous reduction in the independent degrees of freedom. Furthermore, by exploiting the difference in time scale in which the master and the slave amplitudes reach their fixed point solutions, we employ an adiabatic decoupling condition which allows us to analytically describe the system in terms of a fewer effective modes. This leads to an order of magnitude reduction in the computational scaling. A new algorithm is developed based on the synergistic circular causality where only the master amplitudes are determined via coupled cluster theory, while the slave amplitudes are determined either via machine learning or adiabatic decoupling conditions. We will compare and contrast the results by these two complementary approaches. Finally we will present a road-map for including the post-adiabatic corrections.

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Brief Profile: Dr. Rahul Maitra obtained his PhD degree from the Indian Association for the Cultivation of Science, Kolkata in 2013. He had done his post-doctoral research in Princeton University, New Jersey, USA, Cornell University, New York, USA, and RIKEN Center for Computational Sciences, Kobe, Japan. He is presently Assistant Professor, Indian Institute of Technology Bombay, Mumbai since 2018. The major research interests of Dr. Maitra are Quantum Many-body theory of atoms and molecules, Coupled cluster and electronic structure theories, Quantum computing.

Chemical Warta; Vol. 2, No. 2; January 2022
Published by: Indian Chemical Society:
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Young Scientist Conclave Invited Lecture-8 :

Developing dynamic counterion-condensation model to capture ion-localization effect on RNA

Susmita Roy

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The structure and function of RNA are highly responsive to its ion atmosphere in the cellular environment. Among different prevalent metal ions in cellular composition, the physiological presence of Mg^{2+} in addition to a higher concentration of monovalent salt is often found critical in stabilizing an RNA structure¹. We investigate the interplay between a viral RNA triplex pseudoknot structure and ion-atmosphere of such monovalent and divalent ions at an atomic resolution through extensive explicit solvent molecular dynamics simulations and also by developing a Dynamic Counterion-Condensation (DCC) model. Our DCC model is integrated with coarse-grained molecular dynamics simulation. Efficient implicit-explicit coupling schemes between explicit and implicit particles are used to cover the entire range of multiscale phenomena extending Generalized Manning Counter-ion Condensation theory^{2,3}. The model is tested against experimental measurements of the preferential interaction coefficient of Mg^{2+} associated with the RNA. Both explicit and DCC model simulations show, in the presence of Mg^{2+} , a spine of localized hydrated Mg^{2+} to induce a pair of stem-closure where the minor groove between those stems is akin to breathing. Mg^{2+} mediated minor-groove narrowing is coupled with a local base-flipping dynamics of the base-triple which distorts the overall triplex⁴. Developing a coarse-grained DCC model has spurred new possibilities encouraging us to deal with much bigger challenges with large length-scale and long-time-scale phenomena that are associated with RNA regulation beyond the native state.

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Brief Profile: Susmita Roy joined IISER Kolkata as an Assistant Professor at the Department of Chemical Sciences in 2019. She started her research career at IISc, Bangalore, and obtained her PhD in 2015 in Chemistry under the supervision of Professor Biman Bagchi. In 2015, she went to the USA pursuing her post-doctoral research at Rice University, Texas. She also worked as a visiting scientist at Los Alamos National Laboratory, New Mexico from 2017 to 2019. In 2019, she received Har Govind Khorana-Innovative Young Scientist Award



from DBT, Ministry of Science & Technology, Govt. of India. In 2021, she has received CRSI Young Scientist Award from the Chemical Research Society of India (CRSI). She has been appointed as a visiting faculty at the Center for Theoretical Biological Physics (CTBP), Rice University, USA and as an Editorial Board Member of 'Frontiers' from Frontiers in Physics and Frontiers in Molecular Biosciences Journals.













Total List of Awardees



The Convention Awards (including Young Scientist Awards) of the 58th Annual Convention of Chemists, 2021 were awarded to the following Chemists:

1. Analytical Chemistry







Sl. No.	Name of the Award	Name of the Awardee
1.	Professor V. S. Tripathi Award	Dr. Debashree Das, University of Calcutta, Kolkata, debashreedas2@gmail.com 
2.	Professor V. Pandu Ranga Rao Award	Ms. Lakshita Dewangan, Pt. Ravishankar Shukla University, Raipur, lakshitadewangan06@gmail.com 
3.	Professor A. K. Dey Memorial Award	Mr. Pritam Singh, University of Calcutta, Kolkata, singhapritam1994@gmail.com
4.	Indian Chemical Society Research Excellence Award	Ms. Sayantani Mitra, University of Calcutta, Kolkata, syantanimitra020@gmail.com 
5.	Indian Chemical Society Research Excellence Award	Ms. Riya Ghosh, CSIR-CSMCRI, Bhavnagar, riyachem1995@gmail.com 



6.	Indian Chemical Society Research Excellence Award	<p>Dr. G V S R Pavan Kumar, MVGR College of Engineering (A) Vizianagaram, Andhra Pradesh prs_ganti@yahoo.co.in</p> 
7.	Indian Chemical Society Research Excellence Award	<p>Ms. Mousumi Baruah, Shiv Nadar University, Uttar Pradesh mb548@snu.edu.in</p> 
8.	Indian Chemical Society Research Excellence Award	<p>Dr. Nisha Sharma, Himachal Pradesh University, Shimla, nishasharma581@gmail.com</p> 
9.	Indian Chemical Society Research Excellence Award	<p>Mr. Abhishek Katendra, Pt. Ravishankar Shukla University, Raipur abhisekkatendra@gmail.com</p>  <p style="text-align: center;">ABHISHEK KATENDRA</p>
10.	Indian Chemical Society Research Excellence Award	<p>Dr. Indrani Das Sen, Homi Bhabha Centre for Science Education (TIFR), Mumbai</p>  <p>indrani21105@gmail.com</p>

Sl. No.	Name of the Award	Name of the Awardee
1.	Professor A. K. Dey Memorial Award	Ms. Sukanya Paul, Jadavpur University, Kolkata paulsukanya10@gmail.com 
2.	Professor B. C. Halder Memorial Award	Mr. Animesh Kundu, IIT Kharagpur, Kharagpur, West Bengal, animeshkundu@chem.iitkgp.ac.in
3.	Sri B. M. L. Bhasin Memorial Award	Ms. Suvani Subhadarshini, IIT Kharagpur, Kharagpur, West Bengal, suvanicuj@gmail.com 
4.	Indian Chemical Society Research Excellence Award	Mr. Maitrey Chirantan Travadi, The M S University Baroda, Vadodara maitreytravadi12@gmail.com 
5.	Indian Chemical Society Research Excellence Award	Mr. Rakesh Mazumdar, IIT Guwahati rakes176122032@iitg.ac.in  Ms. Riya Mallik, IIT Guwahati mallik@iitg.ac.in 
6.	Indian Chemical Society Research Excellence Award	Ms. Gargi Kundu, NCL Pune gargikundu.ju@gmail.com

7.	Indian Chemical Society Research Excellence Award	<p>Dr. Tatiana V. Safronova, Lomonosov Moscow State University, Moscow, Russia t3470641@yandex.ru</p> 
8.	Indian Chemical Society Research Excellence Award	<p>Ms. Trishnajyoti Baishya, Cotton University, Assam, baishyatrishnajyoti@gmail.com</p> 
9.	Indian Chemical Society Research Excellence Award	<p>Mr. Tanmoy Saha, Jadavpur University, Kolkata tsaha.chemistry@gmail.com</p> 
10.	Indian Chemical Society Research Excellence Award	<p>Ms. Sabeeha Parveen, IIT Kanpur. Kanpur sabeeha@iitk.ac.in</p> 

3. Industrial and Applied Chemistry






Sl. No.	Name of the Award	Name of the Awardee
1.	Indian Chemical Society Award	Ms. Arpita Roy, IIT (ISM) Dhanbad arpitachem28@gmail.com
2.	Professor K R Desai Award	Ms. Shivangi, IIT Ropar, Ropar 2020cyz0005@iitrpr.ac.in 
3.	Indian Chemical Society Research Excellence Award	Ms. Snehalata Saini, IISER Bhopal snehlatasaini@iiserb.ac.in 
4.	Indian Chemical Society Research Excellence Award	Ms. Diksha Sharma, IIT Ropar, Ropar 2018cyz0004@iitrpr.ac.in 
5.	Indian Chemical Society Research Excellence Award	Ms. Nisha Yadav, Amity School of Applied Sciences, Haryana, nishuyadav2017@gmail.com 
6.	Indian Chemical Society Research Excellence Award	Dr. Gurumurthy B R, Ethiopian Technical University, Ethiopia, vogurul@gmail.com 
7.	Indian Chemical Society Research Excellence Award	Dr. G H Gunasekar, IOCL, Faridabad gunasekargh@indianoil.in 

8.	Indian Chemical Society Research Excellence Award	<p>Dr. Amardeep Singh, IOCL, Faridabad singha4@indianoil.in</p> 
9.	Indian Chemical Society Research Excellence Award	<p>Ms. Sonali M Janjal, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad sonalijanjal2009@gmail.com</p> 
10.	Indian Chemical Society Research Excellence Award	<p>Prof. Niraj S Topare, Dr. Vishwanath Karad MIT World Peace University, Pune niraj.topare@mitwpu.edu.in</p> 



4. Organic and Biochemistry





Sl. No.	Name of the Award	Name of the Awardee
1.	Dr. B. N. Mankad Award	Mr. Sovan Niyogi, IISER Kolkata sn19rs046@iiserkol.ac.in 
2.	Dr. J. M. Dasgupta Award	Mr. Vishal Jyoti Roy, IIT Delhi, New Delhi vishalroychemist@gmail.com 
3.	Dr. D. S. Bhakuni Award	Ms. Priyanaka Kataria, CSIR-NCL Pune priyanka.kataria1709@gmail.com 
4.	Professor P. Sengupta Memorial Award	Mr. Sourav Kundu, IISER Bhopal sourav18@iiserb.ac.in 
5.	Professor S. K. Talapatra Award	Mr. Subhamoy Biswas, IIT Guwahati, Assam vandaams93@gmail.com 

6.	Indian Chemical Society Research Excellence Award	<p>Ms. Priyanka Meena, University of Delhi, Delhi ayusheesingh.104@gmail.com</p> 
7.	Indian Chemical Society Research Excellence Award	<p>Mr. Bipin Kumar Behera, IIT Guwahati, Assam bipinkumarbehera2@gmail.com</p> 
8.	Indian Chemical Society Research Excellence Award	<p>Aditi Singh, Marwadi University, Rajkot aditisingh2905@gmail.com</p> 
9.	Indian Chemical Society Research Excellence Award	<p>Mr. Arindam Khatua, IISER Bhopal arindam18@iiserb.ac.in</p> 
10.	Indian Chemical Society Research Excellence Award	<p>Ms. C. Rajalakshmi, CMS College, Kottayam rajalakshmi@cmscollege.ac.in</p> 



5. Physical Chemistry





Sl. No.	Name of the Award	Name of the Awardees
1.	Professor Santi Ranjan Palit Memorial Award	Ms. Ushasi Pramanik, IISER Bhopal ushasi17@iiserb.ac.in 
2.	Professor Santi Ranjan Palit Memorial Award	Ms. Varsha Bharadwaj, The M S University Baroda, Vadodara, varshabhardwaj16@gmail.com
3.	Association of Kineticists Award	Ms. Akansha Chaturvedi, IIT Ropar, Ropar akansha.19cyz0013@iitpr.ac.in 
4.	Association of Kineticists Award	Mr. Mohammedumar Mulla, Karnatak University, Dharwad, umarmulla1985@gmail.com 
5.	Professor S. T. Nandibewoor Award	Mr. Soching Luikham NIT Nagaland sochingluikham@gmail.com 

6.	Indian Chemical Society Research Excellence Award	<p>Mr. Srimanta Pal, IIT Guwahati, Assam srimantapal1994@iitg.ac.in</p> 
7.	Indian Chemical Society Research Excellence Award	<p>Dr. Mousumi Mukherjee, Khalisani Mahavidyalay, Chandannagar, Hooghly, WB mukherjee88@gmail.com</p> 
8.	Indian Chemical Society Research Excellence Award	<p>Mr. Tushar S. Deore, ICT Mumbai ntushardeore@gmail.com</p> 
9.	Indian Chemical Society Research Excellence Award	<p>Dr. Priyanka Purohit, J N V University, Jodhpur pvkinetics@gmail.com</p> 



10	Indian Chemical Society Research Excellence Award	Mr. Vishram D. Hiremani, Karnatak University, Dharwad, vishramhiremani52@gmail.com 
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6. Environmental Chemistry


1.	Dr. Upadhyayulu V. Rao Memorial Award	Mr. Ranadip Goswami, CSIR-CSMCRI, Bhavnagar, iamroni1993@gmail.com 
2.	Dr. Upadhyayulu Annapurna and Satyanarayana Memorial Award	Mr. Ganga Singh, IIT Ropar, Ropar 2018cyz0015@iitrpr.ac.in 
3.	Professor G. Gopalarao Centenary Young Scientist Award	Mr. Mukesh Kumar, IIT Ropar, Ropar 2017cyz0004@iitrpr.ac.in 
4.	Indian Chemical Society Research Excellence Award	Ms. Sukhjot Kaur, IIT Ropar, Ropar sukhjot.19cyz0022@iitrpr.ac.in 

5.	Indian Chemical Society Research Excellence Award	<p>Ms. Amreen K. Bains, IISER Mohali amreenbains06@gmail.com</p> 
6.	Indian Chemical Society Research Excellence Award	<p>Dr. Pragati Fageria, University of Rajasthan, Jaipur, Rajasthan, pragati.fageria@gmail.com</p> 
7.	Indian Chemical Society Research Excellence Award	<p>Dr. Shweta Vyas, University of Kota, Rajasthan shwetavyas@uok.ac.in</p> 

8.	Indian Chemical Society Research Excellence Award	<p>Dr. Gourisankar Roymahapatra, Haldia Institute of Technology, Haldia, West Bengal gourisankar1978@gmail.com</p> 
9.	Indian Chemical Society Research Excellence Award	<p>Ms. K. Vara Lakshmi, GITAM University, Visakhapatnam, vkalla2@gitam.edu</p> 
10.	Indian Chemical Society Research Excellence Award	<p>Dr. Sameer Vyas, Central Soil and Materials Research Station, New Delhi samyog78@yahoo.com</p> 

1.	Indian Chemical Society Research Excellence Award	<p>Ms. Divyani Gupta, IIT Ropar, Ropar 2018cyz0010@iitrpr.ac.in</p> 
2.	Indian Chemical Society Research Excellence Award	<p>Dr. Arti Chouhan, MNNIT Allahabad, Prayagraj artichouhan@mnnit.ac.in</p> 
3.	Indian Chemical Society Research Excellence Award	<p>Prof. Niraj S Topare, Dr. Vishwanath Karad MIT World Peace University, Pune niraj.topare@mitwpu.edu.in</p> 
4.	Indian Chemical Society Research Excellence Award	<p>Dr. Gita Rani, Chaudhary Devi Lal University, Sirsa, Haryana, gtcdlu@gmail.com</p> 
5.	Indian Chemical Society Research Excellence Award	<p>Dr. Arvind K Gautam, NIT Hamirpur, Himachal Pradesh, akgautam@nith.ac.in</p> 

6.	Indian Chemical Society Research Excellence Award	<p>Mr. Amid L. Sadgar, ICT Mumbai amidsadgar@gmail.com</p> 
7.	Indian Chemical Society Research Excellence Award	<p>Dr. Subham Banerjee, NIPER Guwahati subham.banerjee@niperguwahati.ac.in</p> 
8.	Indian Chemical Society Research Excellence Award	<p>Mr. Tapas K. Dutta, IISER Bhopal tapas17@iiserb.ac.in</p> 
9.	Indian Chemical Society Research Excellence Award	<p>Ms. Anu Bala, Chaudhary Devi Lal University, Sirsa, Haryana, ccihag@gmail.com</p> 

10	Indian Chemical Society Research Excellence Award	<p>Mr. Rohit Chatterjee, Haldia Institute of Technology, Haldia, West Bengal roChatterjee01@gmail.com</p> 
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NATIONAL SCIENCE DAY CELEBRATION



Organised by

**Indian Chemical Society
Kolkata**

**Date:
28th Feb
2022**





The pride of Indian Science, Sir. C. V. Raman, discovered the Raman Effect on 28th February, 1928 who worked in the Indian Association for the Cultivation of Science, Kolkata and was awarded the Nobel Prize in 1930. Govt. of India declared in 1987 the 28th February as National Science Day.

Science works for the Benefit of Mankind. Scientific knowledge has led to remarkable innovations that have been of great benefit to the sustainability of the society. Most of the benefits of science are haphazardly distributed although Science does not work for 'Rich' or 'Poor'; Science for all; Science for Self-reliance; Science travels from 'Truth' to 'More Truth' not from 'False' to 'Truth'.

As a part of 'Swadeshi Science Movement' during Azadi ka Amrit Mahotsav the theme of the National Science Day (NSD) 2022 is, "**integrated approach in science and technology for a sustainable future**". The Indian Chemical Society, one of the oldest societies founded by Acharya P. C. Ray as the First President along with J. C. Ghosh, J. N. Mukherjee, S. S. Bhatnagar and others in 1924 is going to celebrate NSD-2022 on 28th February (Monday), 2022 by arranging competitions of Speech, Model and Poster on the Theme topic amongst School children, College/University students and researchers.







This program will be inaugurated by Prof. G. D. Yadav, President, Indian Chemical Society. The Keynote address will be delivered by Prof. Tapas K Das, USA on "*Sustainable Water and Wastewater Treatments: Water Reclamation Technologies for Beneficial Reuse and Recycling*", Dr. T G K Murthy, Former Director, ISRO, Govt. of India will deliver the Special Lecture on "*An overview of India's Space Journey*". Prof. D. C. Mukherjee will introduce the importance of Science Day. Other speakers are Dr. D. V. Prabhu, Founder General Secretary, Association of Chemistry Teachers, Dr. Tapan K Mishra, former Principal, Vidyasagar College, Kolkata and Prof. Ayan Datta, Indian Association for the Cultivation of Science. The students (Class V – PG), young researchers and other dignitaries will present their research on this platform through speech, models and posters.

Participants are requested to fill up the Registration Form (Google form) for participation. **Last date of registration is 25th February 2022.**

This programme will include following competitions

Science Competition (For Students)	<p style="text-align: center;">Group –A: Class V – VI For Speech, Model and Poster: <i>Topic: Save the Biodiversity, Save life / Chemistry & Environment</i></p> <hr style="border-top: 1px dashed black;"/> <p style="text-align: center;">Group –B: Class VII – VIII For Speech, Model and Poster: <i>Topic: Chemistry & Hygiene</i></p> <hr style="border-top: 1px dashed black;"/> <p style="text-align: center;">Group –C: Class IX – X For Speech, Model and Poster: <i>Topic: Water - Crisis and conservation / Plastic – A Boon or A Bane?</i></p> <hr style="border-top: 1px dashed black;"/> <p style="text-align: center;">Group – D: Class XI – XII For Speech, Model and Poster: <i>Topic: Life of C V Raman with reference to Raman Effect / Waste Management at Domestic level</i></p> <hr style="border-top: 1px dashed black;"/> <p style="text-align: center;">Group – E: UG & PG Students of Science & Technology Departments Poster Presentation: - (PPT Presentation, Max. 5 slides, Time 5 min.) <i>Topic: Chemistry in Corona Virus & Treatment / Experience of Learning Chemistry on-line / Green Alternative Energy Sources</i></p>
Research Scholars / Faculty Members	<p style="text-align: center;">Poster Presentation: - (PPT Presentation, Max. 7slides; Time (5+2) min.) Theme: Molecules and Materials : Today and Tomorrow</p>
<p style="text-align: center;">For all Participants: <i>Last date of registration is 25th February 2022 (05:00 pm).</i></p>	

Eminent Speakers

		
Prof. G. D. Yadav President, ICS Kolkata	Prof. C. Sinha Honorary Secretary, ICS	Prof. D. C. Mukherjee Advisor, ICS Kolkata
		
Prof. Ayan Datta Indian Association for the Cultivation of Science	Dr. Thutupalli Gopala Krishna Murthy Ex-Director, ISRO	Dr. D. V. Prabhu, Founder General Secretary, Association of Chemistry Teachers



All Correspondence in connection with the celebration of the National Science Day
2022 may kindly be made at the following E-mail Address

E-mail: nationalscienceday2022@gmail.com

Registration Link: <https://forms.gle/eKuBycZix4KMxPu68>

Communication

Detail: Prof. Chittaranjan Sinha

Honorary Secretary, Indian Chemical Society

Email: ics.correspondence@gmail.com; Mob: 7044231277

Dr. Rahul Bhattacharya

Executive Officer, Indian Chemical Society

Email: nationalscienceday2022@gmail.com; Mob: 9875326565

Registration Fees:

Free for all student participants

Rs. 300/- for Research Scholars, Faculty Members and
Others

NEFT Details


Name of Vendor	Indian Chemical Society
Bank Account Number	11152790242
Nature of Account	Current
Name of Bank	State Bank of India
Branch Name	Manicktala, Kolkata
Branch Code	01715
IFSC Code	SBIN0001715
PAN No.	AAAAL1238H
MICR Code	700002062
IBAN No.	SBININBB492
Vendor Address	92, Acharya Prafulla Chandra Road Kolkata – 700 009
City	Kolkata
Contact No.	033-2350 3478 (Phone & Fax)
E-mail	nationalscienceday2022@gmail.com

PowerPoint Slide Show - [Acharya PC ray memorial award lecture] - PowerPoint

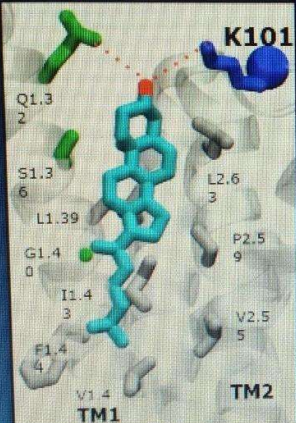
Cholesterol and GPCR Function: A Molecular Sensor for Cholesterol in the Serotonin_{1A} Receptor

Amitabha Chattopadhyay
 CSIR Bhatnagar Fellow
 Centre for Cellular and Molecular Biology
 Hyderabad, India
 amit@cmb.res.in
<http://e-portal.cmb.res.in/e-space/amit/Pages/Index.htm>

Acharya PC Ray Memorial Award Lecture
 Annual Convention, Indian Chemical Society
 December 21, 2021

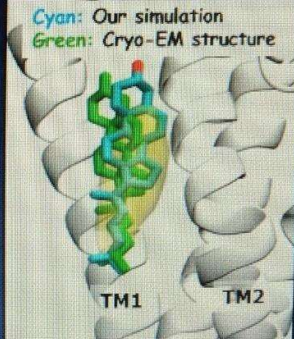


A Molecular Sensor for Cholesterol: Insights from All-atom Molecular Dynamics Simulations




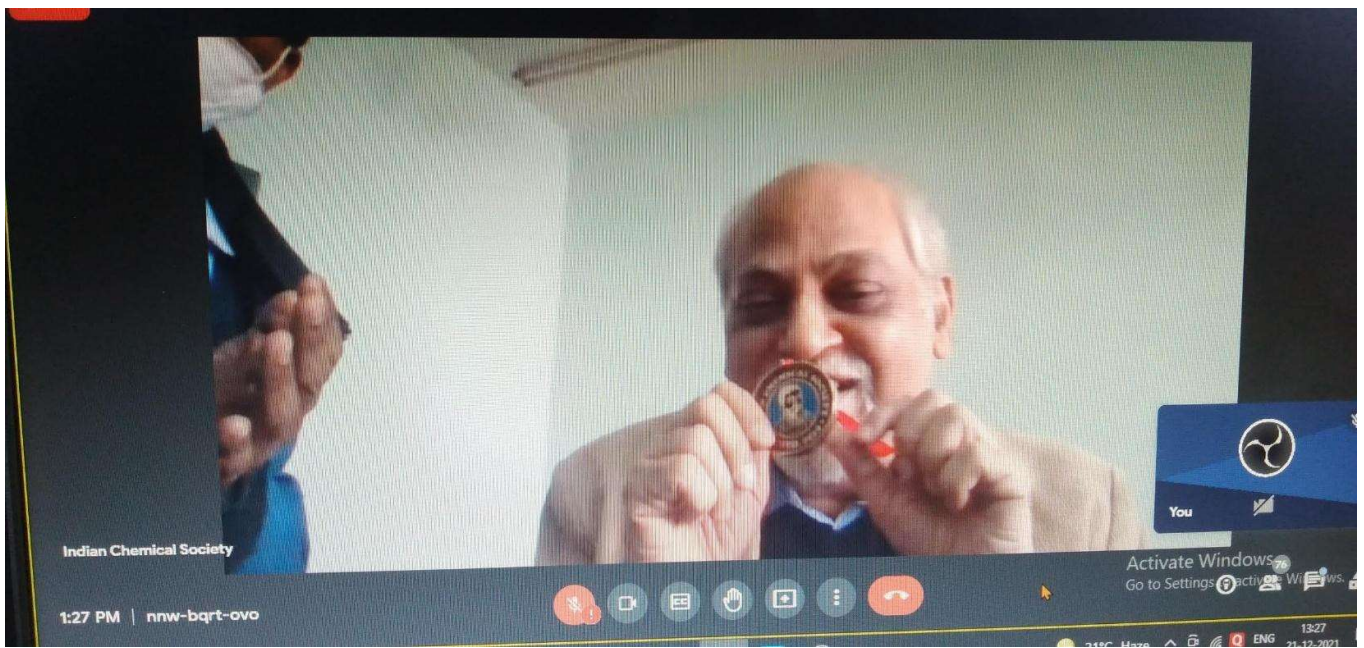
**Cholesterol tightly binds between
TM1 and TM2 by establishing polar
contacts with K101**

Cyan: Our simulation
Green: Cryo-EM structure



**Simulations show a tightly-bound
cholesterol in a position almost identical
to the one observed in the recent
cryo-EM structure**





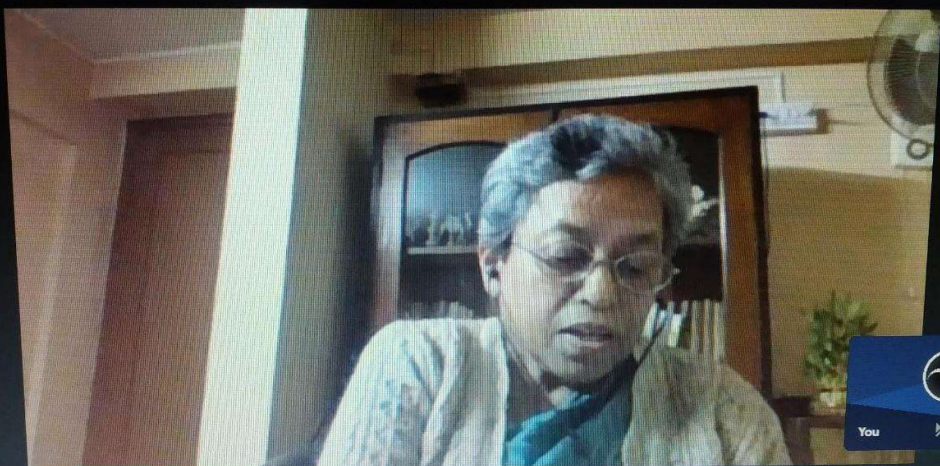
Cooperative effect towards anion binding

Anions	Binding constant in presence of TBA ⁺ (K_{TBA^+} ; M ⁻¹)	Binding constant in presence of K ⁺ (K_K ; M ⁻¹)	K_K / K_{TBA^+}
Cl ⁻	741	1288	1.74
Br ⁻	851	2455	2.88
NO ₃ ⁻	87	324	3.72
HSO ₄ ⁻	501	575	1.15

Highest cooperative effective observed for NO₃⁻

Binding constant follows the same order Br⁻ > Cl⁻ > SO₄²⁻ > NO₃⁻ in presence of K⁺

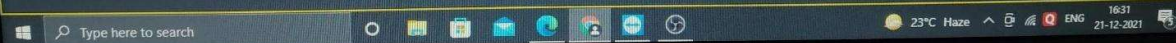
B. Akhuli, P. Ghosh, *Chem. Commun.*, 2015, 51, 16514-16517

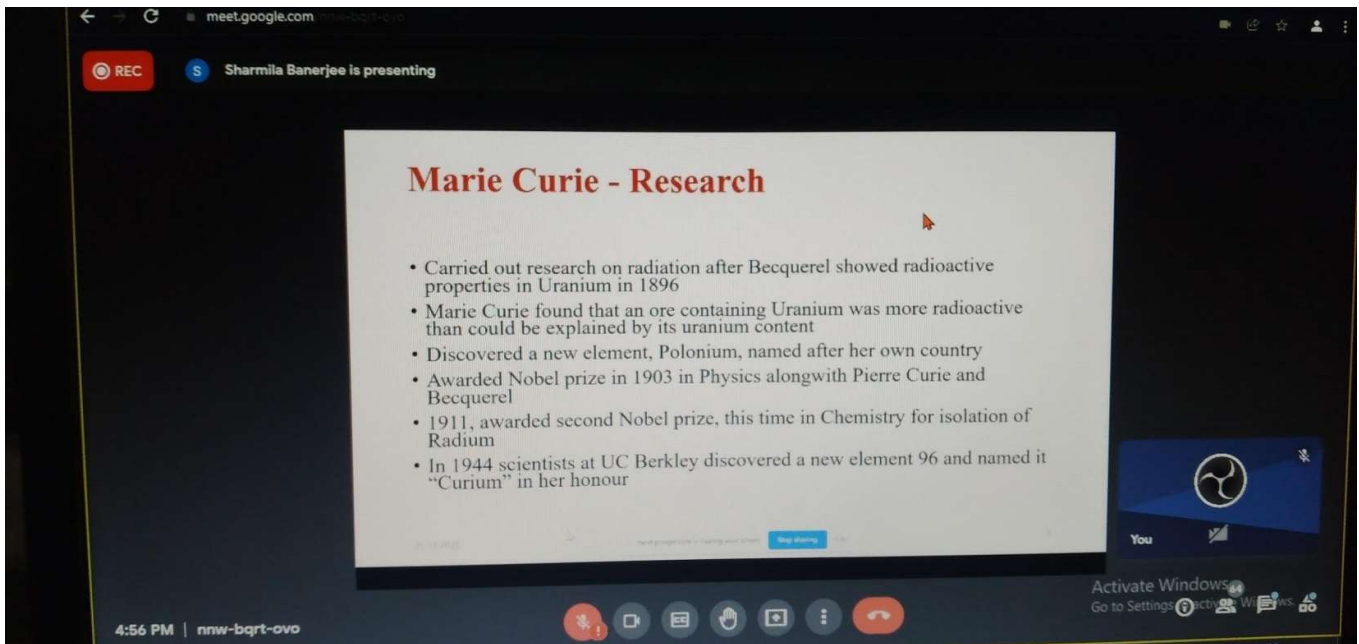
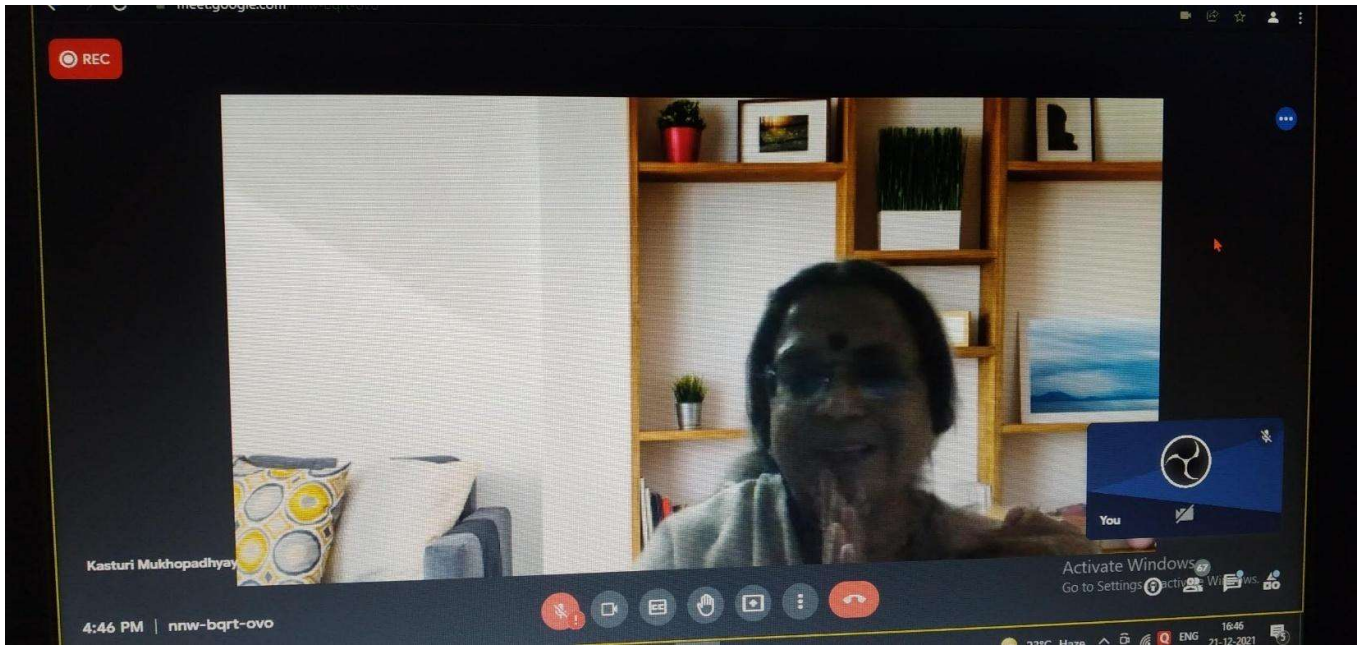


Rina Ghosh

4:31 PM | nnw-bqrt-ovo

Activate Windows
Go to Settings





Akansha Chaturvedi is presenting

9:45 AM | Physical Chemistry Section

19°C Sunny 09:45 22-12-2021

Abhishek Katendra is presenting

Fluorescence Measurements

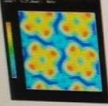
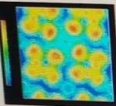
Fig. 4. Plots of intensity ratio I_0/I vs. concentration of antidepressant drugs and presence of various concentration of antidepressant drugs i.e. [A] [Dexam]BF₄+CPZ, [B] [Dexam]BF₄+PMZ, [C] TTAB+CPZ and [D] TTAB+PMZ respectively.

10:06 AM | Physical Chemistry Section

19°C Sunny 10:06 22-12-2021

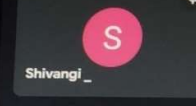
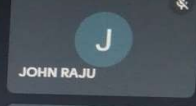
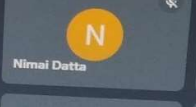
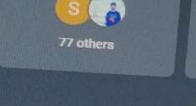

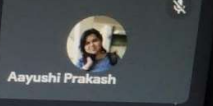


NaAlH₄

- The AlH₄ unit is stabilized by the transfer of one electron from sodium
- The energy needed to remove one hydrogen in the pristine system is 4.0 eV

The energy needed to remove a hydrogen atom in the Ti-doped system is 1.9 eV. > Bond weakening is shown through a stretching of the Al-H bond and from ELF


C. Moyses Araujo, Rajeev Ahuja, and J. M. Osorio Guillén, and Puru Jena, *Appl. Phys. Lett.* **86**, 251913.
 C. M. Araujo, S. Li, R. Ahuja, and P. Jena, *Phys. Rev. B* **72**, 165101.
 S. Li, P. Jena, C. M. Araujo, and R. Ahuja, *Mater. Res. Soc. Symp. Proc. (MRS)* **837**, N2.5.1
 A. Blomqvist, C. M. Araujo, P. Jena, and R. Ahuja, *Appl. Phys. Lett.* **90**, 141904.



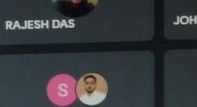
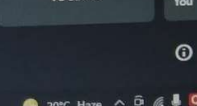




10:28 | RTCS-ENV 2021
 Type here to search
 20°C Haze | ENG | 10:28 22-12-2021

Introduction to Porous Materials

- ✓ A porous medium or a porous material is one which contain pores (voids) typically filled with fluid or gas.
- ✓ Porosity is defined as total pore volume relative to the apparent volume of the material and composition of the material.

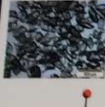


Major Areas of Application

10:47 | RTCS-ENV 2021
 Type here to search
 20°C Haze | ENG | 10:47 22-12-2021

ikaite Crystals grown in the lab




CaCO₃·6H₂O

CaCO₃ precipitate in cold & saturated ice brines
→ hydrated ikaite crystals.

Spectacular ikaite columns (~10 m) discovered around Ikkafofod, southern Greenland. It is difficult to collect ikaite specimen, as the mineral dissolves rapidly under atmospheric conditions into just water and calcite sand!

The crystals found in natural sea ice have a salt-like appearance. **Possibly link to the sea ice-driven carbon pump in ice-covered oceanic waters.**

Ikaite is a strange mineral - plays a key role in the worldwide carbonate deposition and in the global carbon cycle than previously thought. The hydrated calcium carbonate was originally described as a very rare high pressure modification of calcite.



A. Ramanan

A molecular solid

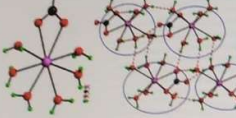
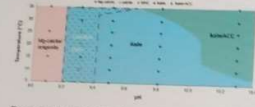
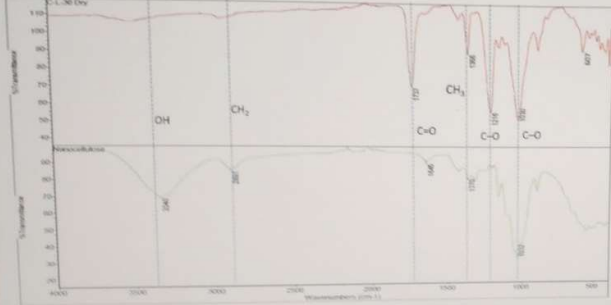




Figure 1. Phase diagram for calcite-celadonite coexistence temperatures as a function of pH in the present solution. In this diagram, four main series have been defined: high salinity (high salinity) series; transition series with pseudomorphs; ikaite series; and ikaite/ACC series. The data represent the results from the experiments with ikaite and the series obtained by others.

Different between Cellulose and Cellulose Acetate (L-30)



The associated stretching of OH groups and the appearance of the ester carbonyl peak at 1737 cm⁻¹ due to O=CO-CH₃ stretching of acetate and the CO stretching of acetyl groups at 1216 and 607 cm⁻¹.




Dr Yoshito Ando

Cellulose Acetate (L-30)

Cellulose

REC
R Riitta Keiski is presenting

Chemistry and Engineering enabling the Energy transition – The role of Catalysis in fostering Sustainability



EU Climate Policy, Ministry of Environment in Finland, 2021. <https://ym.fi/en/eu-climate-policy>
 Government's climate policy, Ministry of Environment in Finland, 2021. <https://mnc.fi/en/climate-neutral-finland-2035>

- Clean air and water essential to human health and the environment
- Global sustainability crisis caused by overconsumption and pollution
- Increasing production and use of energy and more attention to prevent climate change and loss of biodiversity
- Fostering sustainable development (SD) by e.g.
 - New climate policies, sustainable use of natural resources, use of renewable energy, turning to climate-friendly production, reducing the carbon footprint, promoting circular economy
- **Materials and Chemicals for Batteries**
- **Hydrogen as an Enabler of Energy transition**
- **New Materials for Renewable Energy Production**
- **EU policies to guarantee SD**
 - EU's climate policy following the UN Convention on Climate Change, the Kyoto Protocol, and the Paris Agreement
 - Committed to 55% reduction in GHGs by 2030 compared to 1990
 - EU to become the first climate-neutral continent by 2050
 - The European Green Deal (2019)
 - Means to achieve climate neutrality by 2050 and the 2030 target of 55% emissions reduction (the 'Fit for 55' package)
 - Involvement of all citizens and stakeholders in this work
 - **Finland:** Target to become carbon-neutral by 2035 and to be the world's first fossil-free welfare society

Atul Kumar
DIKSHA SHARMA

Debabrasad Mand...
SHAIN KADIR

23 others
You

RTCS-ENV 2021

🔊
🖱️
📺
⋮
📞

Activate Windows
Go to Settings to activate Windows

24°C Haze
14:12
22-12-2021