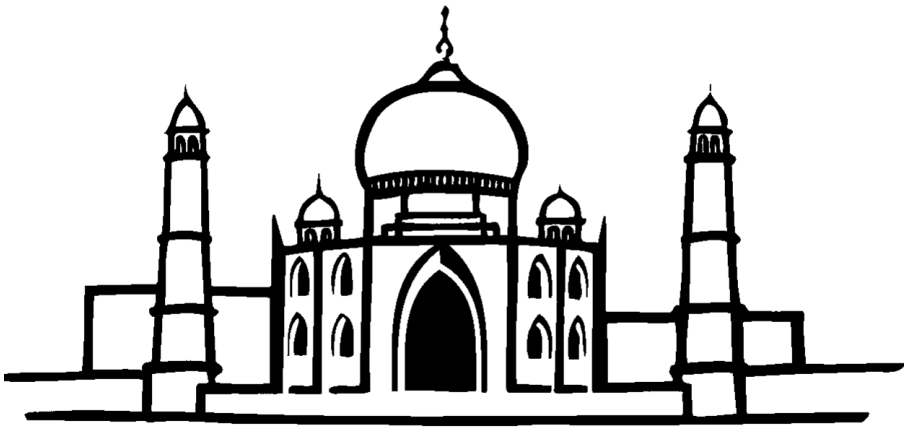
Future Oriented Research Conferences and Exhibitions (FORCE)

Interdisciplinary Initiative in Chemical Sciences (IICS)

FORCE – IICS 2022

ABSTRACTS & BIO-SKETCHES

July 28-31, 2022 at Jaypee Palace, Agra



Co-organized by
IISER Kolkata, IISER Bhopal & IIT Kanpur

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Interdisciplinary Initiatives in Chemical Sciences (IICS) - 2022

From Organizer's Desk

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Interdisciplinary Initiative in Chemical Sciences

Dear Delegates,
Greetings from the Organizing Committee, FORCE-IICS 2022!

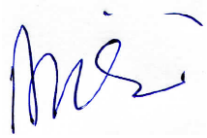
Chemistry has long become a Central Science with multiple major avenues of applications ranging from Drug Discovery, Materials Sciences, Catalysis, Complex Biological Systems and Soft-Robotics etc. Therefore, it is a good idea to have a conference in an interdisciplinary research area where Scientists can meet and exchange ideas on a platform named as Future-Oriented Research Conferences and Exhibitions (FORCE). This conference is to be held at Jaypee palace at Agra based on a theme: 'Interdisciplinary Initiative in Chemical Sciences (IICS)'. We are interested in covering several areas of Chemistry over a span of 3 days, particularly Synthesis, Catalysis, Asymmetric Synthesis, Material Science & Engineering, Energy Storage & Devices, Theoretical Chemistry, Chemical Biology etc.

The FORCE-IICS conference in Chemistry is organized by Indian Institute of Science Education and Research Kolkata (IISERK) during July 28-31, 2022 in association with Indian Institute of Science Education and Research Bhopal (IISERB) and Indian Institute of Technology Kanpur (IITK). The organizing committee of FORCE-IICS takes the pleasure of inviting you to this symposium. The symposium includes invited lectures, and special lectures by eminent chemists and scientists working in the allied areas of chemistry from our Country. The FORCE-IICS provides a platform for scientists, and faculty members to discuss the recent developments in chemical sciences across the sub-disciplines.

In addition, FORCE-IICS creates opportunities to exchange ideas and to build long lasting collaborations in the frontier areas of chemistry and its allied disciplines. There will be a 'Special Evening Lecture' by Prof. G. Mehta on 'Sustainability' and panel discussion on "Repurposing Research: Fostering Interdisciplinarity", where Prof. Shekhar C. Mande, Ex-DG, CSIR and Prof. Ashutosh Sharma, Ex-Secretary, DST will speak and other eminent personalities including Prof. Sourav Pal, Prof. Vinod K. Singh, Prof. Ganesh Pandey, Prof. Uday Maitra, Prof. Sandeep Verma, Prof. G. Mugesh and others will express their views.

We hope that you will enjoy this episode of celebration of Chemistry and at the same time enjoy the rich heritage of Agra including the *Taj Mahal!*

Yours Sincerely,



Alakesh Bisai
Convener, FORCE-IICS 2022

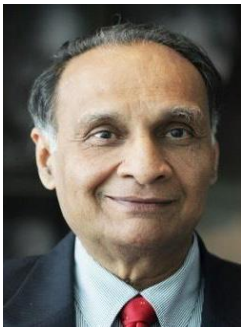
Bio-Sketch of Speaker of 'Special Evening Lecture'

Bio-Sketch – Special Evening Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

…Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker



Goverdhan Mehta
Professor, FRS
University Distinguised Professor &
Dr. Kallam Anji Reddy Chair
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Prof. Goverdhan Mehta, FRS, is a leading chemist of our times. Prof. Mehta's design of complex molecules blends art and architecture and has culminated in more than 450 original research papers in international journals of high repute. Today "Chemistry can re-imagine itself as a champion and driver of sustainable development, transforming its image from often being seen as the source of environmental pollution and degradation to being recognized as the core sustainability science, "Prof. Mehta is one of those few to whom we owe this change of public perception of chemistry as a central and sustainable science.
Prof. Goverdhan Mehta received his MSc Chemistry degree from BITS Pilani, in 1963. A PhD from Poona University working at National Chemical Laboratory with legendary Dr. Sukh Dev, he has been conferred over a dozen Honorary Doctorate (D. Sc. h. c) degrees by universities in India and abroad, he started his academic career at IIT Kanpur before moving to University of Hyderabad, where he went on to become the Vice-Chancellor and later he became the Director of IISc Bangalore. Apart from these responsibilities Prof. Mehta has furthered the cause of Indian Academia by serving as Chairman, National Accreditation and Assessment Council (NAAC), Chancellor, Indian Institute of Information Technology, Allahabad, Chancellor, University of Allahabad, Chairman, BoG, Indian Institute of Technology, Jodhpur, Chairman, Indian Statistical Institute Council, Board of Directors, Institute of Life Sciences and several other key positions of trust and critical importance. As an organic chemist Prof. Mehta has created NCE's for drug discovery, origin and control of stereogenesis, engineered conformationally locked polyols and photodynamic therapy of cancer, and has moved to major policy making where he has profiled and promoted chemical sciences as 'sustainability science'.

Prof. Mehta's contribution to science has been honored with numerous national and international civilian accolades of highest orders ranging from "Padma Shri" (India), "Légion d'honneur" (France), to "Bundesverdienstkreuz" (Germany). He is also the recipient of the Centenary Prize (2005), the first Indian scientist to receive the Alexander von Humboldt Research Award (1995), G.D. Birla Award for Scientific Research, and Shanti Swaroop Bhatnagar Award in Chemical Sciences to name a select few. Apart from being a Fellow of the Royal Society (FRS) and the National Academics of Sciences in India, Prof. Mehta is the past president of IUPAC, INSA, and a foreign member of the Russian Academy of Sciences. Prof. Mehta's keen enthusiasm for chemistry has inspired many to take up this profession. In spite of being cradled with creativity and success, his laughter and humor is contagious, crystallized with a clarity of mind and modesty. Prof. Mehta makes us remember to have the wisdom to walk with crowds and yet not loose touch of the kings of knowledge. He, like the Zeus, has been morphing Chemical Sciences in his sleeves and crucibles, just with a toss of his hand and touch of his creative discipline. His name is synonymous to an institution in synthetic chemistry of our times and beyond.

Bio-Sketch of Members of the 'Advisory Council' of the FORCE-IICS Conference 2022

Bio-Sketch

Sourav Pal
Professor & Director
IISER Kolkata

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Prof. Sourav Pal is Director of Indian Institute of Science Education and Research (IISER) Kolkata on deputation from Indian Institute of Technology (IIT) Bombay. He was formerly the Director of CSIR-National Chemical Laboratory (NCL), Pune and worked at NCL Pune for almost 33 years. He was instrumental in setting up Electronic Structure Theory Group at NCL. He is a distinguished theoretical chemist and has contributed to methodological and conceptual developments on many-body electronic structure theory, to the area of density based chemical reactivity, as well as to catalytic and hydrogen storage materials using computational material science.

With masters degree in Chemistry from Indian Institute of Technology (IIT) Kanpur in 1977, and a Ph.D. degree from Calcutta University, he joined NCL in 1982. He was a post-doctoral fellow at the University of Florida, Gainesville, USA (1986-87) and Alexander von Humboldt Fellow at the University of Heidelberg, Germany (1987). He was visiting Professor at the University of Arizona, Tucson, USA, University of Torun, Poland and the Institute for Molecular Sciences, Okazaki, Japan. He also holds Adjunct professorships at IISER Pune and IIT Goa. He is also distinguished Visiting Professor at IIT Kharagpur. He served as the President of Chemical Research Society of India for three years from April 1, 2014. He is a member of Executive Council of Federation of Asian Chemical Societies and is Chairman of Chemical Division Council of Bureau of Indian Standards. In addition, he has served on several important scientific committees in the country. He is a member of the Council of Indian National Science Academy, New Delhi.

He has received several awards and honours in recognition of his contributions to science, including the prestigious Shanti Swarup Bhatnagar Award in Chemical Sciences in 2000 and SASTRA-CNR Rao Award in Chemistry & Materials Science in 2014. He is a Fellow of The Indian National Science Academy (2003), Indian Academy of Sciences (1996) and National Academy of Sciences (1998), and the Maharashtra Academy of Sciences (1994). He is J C Bose National Fellow of Department of Science and Technology from 2008. He is a Fellow of the Royal Society of Chemistry, U.K. (2011).

He is on the Editorial Advisory Board of the Journal of Physical Chemistry and has published about 270 papers in international peer-reviewed journals and contributed chapters to several books. He has guided more than 35 Ph.D. theses and is the author of a book titled "Mathematics in Chemistry".

Bio-Sketch

Vinod K. Singh
Chair Professor
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Professor Vinod Singh is currently Rahula and Namita Gautam Chair Professor at IIT Kanpur. He is also Director's Chair Professor at IISER Bhopal & adjunct Professor at NIPER Hyderabad. He is currently the President, Chemical Research Society of India (CRSI) and the Chairperson, Governing Council of IACS Kolkata.

Born on 9th September, 1959 in Anantpur, a village near Nizamabad in the district of Azamgarh (U.P.), Vinod Singh had his early education from his native place. He passed high school and intermediate from Wesley Inter College and B.Sc. (1978) from D.A.V. College, all from Azamgarh. He did M.Sc. in Chemistry from B.H.U. (1980) and Ph.D. under the guidance of Dr. Sukh Dev from Malti-Chem Research Center, Nandesari, Baroda (Degree awarded in 1986 by M.S. University). He was conferred upon D.Sc. (honoris causa) by Jabalpur University in 2012. Professor Singh spent 2 years for his postdoctoral work in Canada (1985-1987) at the University of Calgary and the University of British Columbia. He subsequently moved to the U.S.A. to do other postdoctoral work (1987-1990) at Harvard University with Professor E. J. Corey, a Nobel Laureate. After a brief stint as a Senior Scientist at Neurogen Corporation, CT, USA, Vinod Singh joined IIT Kanpur in 1990 as an Assistant Professor and rose to the rank of Professor. Professor Singh's research falls in the area of Synthetic Organic Chemistry, more specifically, asymmetric synthesis.

He has been recognized with several awards and honours such as Swarnajayanti Fellowship (1998), Shanti Swarup Bhatnagar Prize (2004) and Padma Shri (2014), among others. In addition, he has been elected as a Fellow of the Indian National Science Academy (FNA), Indian Academy of Sciences (FASc), National Academy of Sciences (FNASc), and The World Academy of Sciences (FTWAS). Professor Singh is an Editor of an Elsevier journal - *Tetrahedron Lett.* He is a Member, Editorial Advisory Board of *Org. Lett.* and *J. Org. Chem.*, *Asian J. Org. Chem.*, and *Org. Chem. Frontiers*.

He has made significant contributions in the management of higher educational institutes, science education, science policy, and planning. In 2020, he was awarded a TWAS-CASAREP award for building scientific institutions. As a Founding Director of IISER Bhopal for more than 10 years (2008-2018), Professor Singh set up the whole campus in 200 acres of land from scratch. He has served as the Mentor Director of IISER Berhampur, Director of SPA Bhopal (additional charge) and the Chairman of BoG, NITTTR Bhopal. He also held the additional charge of Directorship of MANIT Bhopal and the Mentor Director of IIIT Bhopal. Professor Singh had been a Member of the Scientific Advisory Council to the Prime Minister (SAC to PM) during 2009-2014.

Bio-Sketch

G. Mugesh
Professor of Chemistry
Department of Inorganic & Physical Chemistry
IISc Bangalore

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Prof. G. Mugesh received his B.Sc. (1990) and M.Sc. (1993) degrees from the University of Madras and Bharathidasan University, respectively. He obtained his Ph.D. (1998) at the Indian Institute of Technology, Bombay, under the supervision of Prof. H. B. Singh. In 2000, he moved to Germany as an Alexander von Humboldt Fellow at the Technical University, Braunschweig. In 2001-2002, he worked with Prof. K. C. Nicolaou at the Scripps Research Institute, as a Skaggs postdoctoral fellow.

His work ranges from fundamental chemical synthesis and reaction mechanism at the molecular level to practical biomedical applications. His work on artificial enzymes including nanozymes that modulate the cellular redox signalling has attracted a global attention. The recent discovery from his laboratory that proteins and small molecules can be delivered into mammalian cells by utilizing halogen bonding has direct applications to human health. This novel strategy can be used for the efficient delivery of proteins and small molecules for therapeutic applications.

He is a recipient of Infosys Prize in Physical Sciences (2019); CRSI Silver Medal (2019); National Prize for Research on Interfaces of Chemistry and Biology (2017); Rajib Goyal Prize in Chemical Science (2017); Bhagyatara Award (2017); ISCB Award for Excellence (2016); J. C. Bose National Fellowship (2015); Shanti Swarup Bhatnagar Prize (2012); AstraZeneca Excellence in Chemistry Award (2012); CDRI Award for Excellence in Drug Research (2010); Swarnajayanti Fellowship (2006-07); Ramanna Fellowship, DST (2006).

He is a fellow of the National Academy of Sciences, India (2012), Indian Academy of Sciences (2012) and Indian National Science Academy (2016). He currently serves as Vice-President of the Chemical Research Society of India (CRSI). He has served as the Secretary General of the Chemical Research Society of India (CRSI) and also as President of the Asian Chemical Editorial Society (ACES). He also serves in the Editorial or Editorial Advisory Boards of Chemistry – A European Journal (ChemPubSoc, Europe), Organic and Biomolecular Chemistry (RSC), ACS Omega (ACS); Bioorganic Chemistry (Elsevier) and Biological Chemistry (De Gruyter, Germany).

Bio-Sketches of Speakers of 'Expressing Views in the Interdisciplinarity in Sciences'

Bio-Sketch of Speaker

Ganesh P. Pandey
Distinguished Professor, BHU
& Ex-Director, CBMR Lucknow

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Banaras Hindu University

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Homepage: https://new.bhu.ac.in/Site/FacultyProfile/1_150?FA001039

Ganesh Pandey studied Chemistry at Banaras Hindu University, Varanasi, India. After completing his Ph. D. in 1980, he proceeded to Purdue University, U.S.A. for his post- doctoral studies in the group of Prof. Harry A. Morrison where he studied the photobiology of urocanic acid, the skin pigment. On returning to India in mid-1983, he first joined Panjab University, Chandigarh as a CSIR "Pool Officer" and within six months moved to Indian Institute of Chemical Technology, Hyderabad as a Scientist and continued there until July 1991. He moved again to National Chemical Laboratory, Pune in 1991 and continued there until February 2013. He again moved as a Director of Centre of Biomedical Research, Lucknow in 2013 and continued there till February 2019.

His research interest continues in the area of the total synthesis of natural products, development of newer synthetic methodologies, asymmetric synthesis and radical-ion chemistry and drug discovery.

Prof. Pandey is recipient of some of the most prestigious prizes in India such as Shanti Swarup Bhatnagar Prize, J. C. Bose Fellowship, P. C. Ray Memorial award and Goyal Science Prize. He is the Fellow of all the three National Science Academies of India. He also served as Editor of *Tetrahedron* and an Editorial Board Member for *Asian J. Org. Chem.* and *Chinese Chem. Lett*.

Bio-Sketch of Speaker

Uday Maitra
Professor

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Homepage: https://orgchem.iisc.ac.in/uday-maitra/

After his BSc from Presidency College, Calcutta and MSc from IIT Kanpur, Uday Maitra received his M. Phil and PhD from Columbia University in 1986 working with Prof. Ronald Breslow. Following a postdoctoral stay at the University of California at Berkeley with Prof. Paul Bartlett, he returned to India, and after a year at IIT Kanpur moved to IISc Bangalore in 1989.

His research interests are in the Chemistry of Bile acids; Hydrogels, Metallohydrogels and Organogels; Organic-inorganic hybrid materials; Enzyme sensing, etc. His group has recently developed a general strategy for low cost, paper-based photo-luminescent enzyme sensors. He is also greatly interested in Chemistry Education and is a regular participant in a variety of outreach programmes for high school and undergraduate students

Bio-Sketch of Speaker

Sandeep Verma
Secretary, SERB India
Shri Deva Raj Chair Professor
Department Of Chemistry
DST Unit of Excellence on Soft Nanofabrication
Center for Environmental Sciences and Engineering
Indian Institute of Technology Kanpur

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Homepage: http://home.iitk.ac.in/~sverma/

Sandeep Verma is an Indian bioorganic chemist and chemical biologist, and a Professor in the Department of Chemistry at the Indian Institute of Technology, Kanpur (IITK).

Born on 24 June 1966, in Kanpur in the Indian state of Uttar Pradesh, Sandeep Verma did his early schooling in Varanasi and completed his master's degree at Banaras Hindu University in 1989. He completed his doctoral work from University of Illinois Medical Center, Chicago (1994), followed by postdoctoral stints at Johns Hopkins Medical Institutions, Baltimore, USA, and at Max-Planck-Institute for experimentelle Medizin, Goettingen, Germany. He joined Department of Chemistry, Indian Institute of Technology Kanpur, in 1997, where he currently holds the positions of Professor of Chemistry and Shri Deva Raj Endowed Chair Professor. He is also an affiliated faculty in DST Thematic Unit of Excellence on Soft Nanofabrication and Center for Environmental Science and Engineering, at IIT Kanpur.

His work has been recognized by DAE-SRC Outstanding Investigator Award (2012), Shanti Swarup Bhatnagar Prize in Chemical Sciences (2010), CDRI Award for Excellence in Drug Research (2009), Swarnajayanti Fellowship (2005), B M Birla Science Prize (2004), to name a few. He is an elected Fellow of Indian Academy of Sciences and National Academy of Sciences, India, and also a Senior Fellow, The Zukunftskolleg, University of Konstanz, Germany. He serves on the editorial advisory boards of Chemical Communications, Chemistry & Biology and Journal of Chemical Sciences. His research interests include metal-nucleobase interactions, peptide/protein self-assembly, and programmable soft matter.

Sandeep Verma is currently serving as the secretary, Science and Engineering Research Board (SERB).

Bio-Sketch of Speakers for 'Panel Discussion' on "Repurposing Research: Fostering Interdisciplinarity"

Bio-Sketch of Speaker

Shekhar C. Mande
Ex- Director General
CSIR, India

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Webpage:
https://en.wikipedia.org/wiki/Shekhar_C._Mande

Dr. Shekhar C. Mande is an Indian Structural and Computational Biologist. He is the ex-Director General of the Council of Scientific and Industrial Research (CSIR), India, and the ex-Secretary of the Department of Scientific and Industrial Research (DSIR), Ministry of Science and Technology. Prior to this, he was the Director of National Centre for Cell Science, Pune.

Dr. Shekhar Mande did his M.Sc. in Physics from University of Nagpur and holds a doctoral degree in Molecular Biophysics from the Indian Institute of Science (IISc), Bengaluru. Following his PhD, he joined Prof. Wim G. J. Hol as Post-Doctoral Fellow at Rijksuniversiteit Groningen in the Netherlands in 1991 and in 1992 joined as a senior fellow at the University of Washington, Seattle, USA.

On his return to India, Dr. Shekhar Mande joined the CSIR-Institute of Microbial Technology, Chandigarh, as a scientist and in 2001 was selected as a Staff Scientist at the Centre for DNA Fingerprinting and Diagnostics, Hyderabad. In 2011, Dr. Mande was appointed as the Director of NCCS, Pune. Dr. Mande has served in various advisory committees for the Government of India.

In 2005, he was awarded the Shanti Swarup Bhatnagar Prize for Science and Technology – the most prestigious science award in India – in the category of Biological Sciences. He has been honoured with several other prestigious awards including the B M Birla Young Scientist Award in 1999, and Wellcome Trust International Senior Fellow 2003-08. He has been elected Fellow of all the three major science academies in the country – the Indian National Science Academy (INSA), National Academy of Sciences, India (NASI), and the Indian Academy of Sciences (IAS). He is also Life member of the Indian Crystallographic Association, the Indian Science Congress Association and the Indian Biophysical Society. Dr. Mande is also credited with the BC Guha Memorial Lecture of the Indian National Science Academy, 2017 and the BK Bachhawat Memorial Lecture of the National Academy of Sciences, India, 2017.

Bio-Sketch of Speaker

Ashutosh Sharma
Ex-Secretary, DST India
Institute Chair Professor &
INAE Visvesvarya Chair Professor &
Coordinator, DST Unit on Nanoscience &
Center for Environmental Science and Engineering
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Dr. Ashutosh Sharma (born 1961) is an Institute Chair Professor and C V Seshadri Chair Professor at the Department of chemical engineering of Indian Institute of Technology Kanpur. He is the founding Coordinator of DST Thematic Unit of Excellence on Soft Nanofabrication and Chairman of Centre for Environmental Science and Engineering at IIT Kanpur. He is best known for his pioneering research work in the areas of colloids, thin film, interfaces, adhesion, patterning and in the fabrication and application of self-assembled nano-structures.

Ashutosh Sharma got his B.Tech degree in Chemical Engineering from Indian Institute of Technology Kanpur (IIT Kanpur), India in 1982. He graduated with master's degree from Pennsylvania State University in 1984 and three years later obtained his Ph.D. in Chemical Engineering from the University at Buffalo, where he worked with Prof Eli Ruckenstein.

He is an elected fellow of prestigious societies such as the Academy of Sciences for the Developing World, Indian National Science Academy, Indian National Academy of Engineering, Indian Academy of Sciences and the National Academy of Sciences, India. In 2002, he received Shanti Swarup Bhatnagar award in engineering sciences for his "original pioneering contribution to the understanding of the behaviour of thin films and other highly confined nanoscale systems". In the next year, he was awarded Herdillia Award by the Indian Institute of Chemical Engineers. In the year of 2010, Infosys Science Foundation have awarded him with Infosys Prize in Engineering and Computer Science for his "scholarly scientific contributions in the broad areas of nanoscale surface pattern evolution, instability, and the dynamics of thin liquid and solid films and soft matter.". He is also a recipient of the 2008 TWAS Prize for his pioneering work on colloids, film interfaces, adhesion etc.

He was a member of the editorial board of Chemical Engineering Science, served on the editorial board of the Journal of Colloid and Interface Science (2000-2002) and Canadian Journal of Chemical Engineering (2006-2008). He was in the editorial board of Nanomaterials and Energy journal. He served as an Associate Editor of the Journal of Micro - and Nano-Manufacturing. From 2013 to date, he has been serving as an Associate Editor of ACS Applied Materials & Interfaces journal.

Chairpersons & Speakers of the Technical Sessions
FORCE - IICS - 2022

Bio-Sketch of Convener

Alakesh Bisai
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Alakesh obtained his Ph.D. under the supervision of Professor Vinod K. Singh from IIT Kanpur in Sept. 2006. Immediately afterward, he moved to UC Berkeley, where he held postdoctoral position with Professor Richmond Sarpong. In Dec. 2009, he left Berkeley and joined IISER Bhopal as an Assistant Professor and rose to the rank of Professor of Chemistry continued his Academic journey till May, 2020. Later, he moved to the Department of Chemical Sciences, IISER Kolkata. The research focus of the AB research group includes the total synthesis of architecturally interesting biologically active natural products that provide an ideal platform for the invention of new oxidative strategies and highly selective organic transformations. His total synthesis of pyrrolo/furoindoline alkaloids has been highlighted in '*Organic Chemistry Portal*' as '*The Bisai Synthesis of (-)-Physovenine*'. His research has been appreciated in various forms, to name a notable one:

CDRI Award in 2022 (Excellence in Drug Research)
Silver Medal, Chirantan Rasayan Sanstha, VU (2021)
Bronze Medal, Chemical Research Society of India (2021)
Fellow, Indian Chemical Society (FICS-2020)
SERB-STAR Award (2020-2023)
CRSI Young Scientist Award (2018)
DST Young Scientist Research Grant (2013)
BRNS Young Scientist Award & Grant (2011)
GRC Award to Postdoc. by Chair, 17th GRC on Stereochemistry (2008)
Postdoc. Fellowship, UC Berkeley (2006-2009)

He delivered several invited lectures in India and abroad, to name a few,

OCS, IIT Kanpur (2022); *FSCHM*, IISER TVM (2022); *RSC-IISER Desktop*, IISER Mohali (2021); *LIMA*, Strasbourg & Mulhouse (2021); *FloHet*, Univ. of Florida (2020); *RACMS*, Indian Chemical Society (2020); Georgetown Univ. (2020); *ICOC*, Goa (2020); *MedChem*, IIT Madras (2019); *OMSRI*, IIT Roorkee (2019); *SERB-VORTEX*, IIT Bombay (2019); *OCS*, IIT Kanpur (2018); *NOST-OCC* (2018); *ISNSCON*, Vigyan Bhawan (2018); *ICOC*, Holiday Inn, Goa (2018); *RAOBC*, IISER Mohali (2018); *BASF*, Mumbai (2017); *AOC*, CSIR-NCL Pune (2017); *11th CRSI-RSC*, Gauhati Univ. (2017); IIT Indore (2017); *ICOS-21*, IIT Bombay (2016); *FICS*, IIT Guwahati (2016); *Pfizer Symposium*, IISc Bangalore (2016); *9th CRSI-RSC*, Punjab Univ. (2015); *INDIGO (Indo-German)*, Univ. of Regensburg (2015); *BASF*, Ludwigshafen (2015); *NFCFA*, BITS Goa (2015); *IICM*, IISER TVM (2015); *INDIGO*, Mahabalipuram (2014); *IGCBIC (Indo-German)*, IISc Bangalore (2014); *RSC-IISER Bhopal* (2013); *NOST-OCC* (2012); *Gregynog Synthesis Workshop*, Univ. of Wales (2011); Univ. of Bath (2011); Cardiff Univ. (2011).

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch

Sangit Kumar
Professor & Head
Department of Chemistry
IISER Bhopal

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E-Mail: sangitkumar@iiserb.ac.in

Group Homepage:

Sangit is a Saharanpur native - born and raised. He attended Chaudhari Charan Singh University, Meerut in 1995 for Bachelor degree and then University of Roorkee (now IIT Roorkee) for Masters in Chemistry in 1999. Supported by UGC CSIR, he attended IIT Bombay in 2002 for his Ph.D. studies under the supervision of Professor H. B. Singh.

He then carried out post-doctoral research with Professor Lars Engman and Professor Michael R. Detty at the Uppsala University, Sweden and University of Buffalo, Buffalo, NY, US. In 2007, Sangit has was awarded by prestigious international Japan Society for Promotion of Science (JSPS) fellowship. Excited to return to India, Sangit began his independent research career in 2009 at IISER Bhopal as an Assistant Professor. He was promoted to Associate Professor in 2013, and to Full Professor in 2018. After starting his independent research carrier, Sangit has published 81 research article and 2 book chapters. Till now, Sangit has guided 10 Ph.D. students, one intergrated Ph.D. student, 15 MS students, and 3 post docs. Currently, he is guiding 8 Ph.D. students, 3 MS students, 1 project student, and 2 post-docs.

He is also an active member of American Chemical Society, Life Member of Society for Materials Chemistry, Chemistry, BARC Mumbai, and Life Member of Chemical Research Society of India (CRSI), Bangalore. His main research interest lies in the group 16th elements: sulfur, selenium and tellurium chemistry. Synthesis of organochalcogens is the main focus in his research group. Exploration of catalytic properties for examples antioxidant and oxidant properties in the context of biomemitics study, electrocatalysts and catalysts for organic transformations is the another research theme in the group.

Adaptive Soft Molecular Crystals

C Malla Reddy*
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Abstract:
High crystallinity, although desired in materials for a wide range of high-performance engineering applications, generally it comes with undesirable attributes such as high brittleness and fragility.1 This makes crystalline materials incompatible with many future technologies, such as flexible devices and soft-robotics. Recent progress in crystal engineering has brought into light many possible opportunities to address these issues, enabling the design of adaptive crystalline materials that respond to external stimuli with exceptional qualities.1-7 For instance, crystals that bend (elastically or plastically), twist, curl, wind, jump, exfoliate, laminate, and explode, under external stresses, such as mechanical stress, pressure, light, heat, solvent, etc., have been shown. On the other hand, until very recent times, self-healing was observed only in soft and amorphous materials, mostly involving approaches that use chemical reactions, diffusion, solvent, vapour, electricity, etc., with typical healing time scales in minutes to weeks.8 A new self-healing mechanism that we recently introduced9 in materials science, enables ultrafast, near 100% autonomous diffusion-less repair in crystalline materials that uses electrostatic surface potentials generated on the freshly created fracture surfaces, inherent to certain types of non-centrosymmetric single crystals. My talk will cover structure-property correlation for crystal engineering of adaptive soft crystals.

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3. Ghosh, S. & Reddy, C. M. (2012) Angew. Chem. Int. Ed., 51, 10319.
4. Krishna. G. R., Devarapalli, R., Lal, G. & Reddy, C. M. (2016) J. Am. Chem. Soc., 138, 13561.
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Bio-Sketch of Speaker

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Dr C Malla Reddy is a Professor and Head at the Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata. His research work focuses on building strong capability in interdisciplinary areas of fundamental and applied Crystal Engineering. His group is credited for the pioneering work on mechanically flexible molecular crystals, structure−mechanical property relationship and also contributed to the concept of self-healing in single crystals. Dr Reddy obtained his PhD from University of Hyderabad and took up Post-doctoral Research at the Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany (2007 – 2008). Dr Reddy has been awarded with Swarnajayanti Fellowship in Chemical Sciences for the year 2015, by the Department of Science and Technology, Government of India and Bhagyatara award for the year 2019 from University of Punjab. He has published more than 100 peer-reviewed research articles. Currently, he is serving as an Associate Editor for CrystEngComm by RSC and co-editor for Acta Crystallographica Section B. He was an Associate Editor for RSC Advances during 2015-16.

References and Notes:

(1) S. Bhunia, S. Chandel, S. K. Karan, S. Dey, A. Tiwari, S. Das, N. Kumar, R. Chowdhury, S. Mondal, I. Ghosh, A. Mondal, B. B. Khatua, N. Ghosh, C. M. Reddy, **Science,** 2021, *373*, 6552, 321-327.
(2) A. Mondal, B. Bhattacharya, S. Das, S. Bhunia, R. Chowdhury, S. Dey and C. M. Reddy, **Angew. Chem. Int. Ed.**, 2020, *59*, 2-12.
(3) Krishna, G. R., Devarapalli, R., Lal, G., Reddy, C. M., **J. Am. Chem. Soc.** 2016, *138*, 13561−13567.
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Biochemical Investigation of a Hydrocarbon-Producing Metalloenzyme

Tabish Iqbal, Subhashini Murugan, and Debasis Das*
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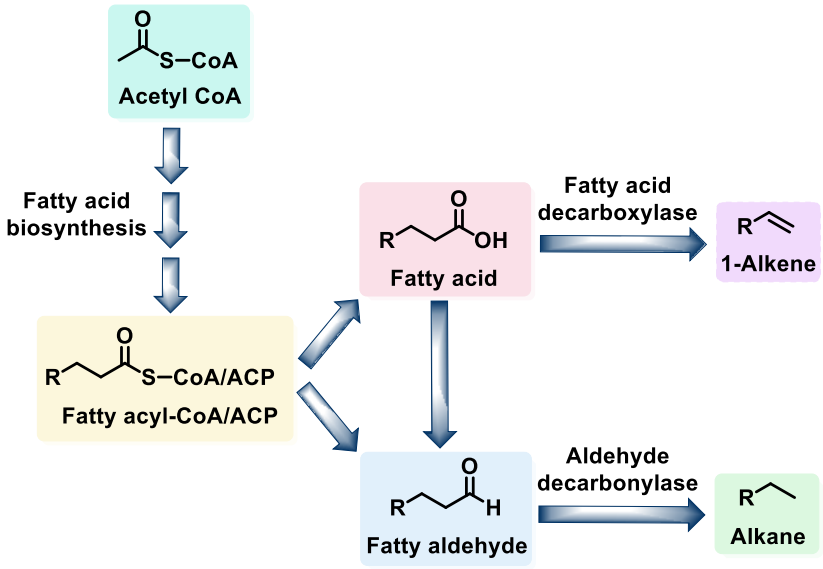
Abstract:
The increasing concerns of global warming associated with the usage of fossil fuels have sparked intense interest in developing renewable, eco-friendly fuels known as biofuels. Simple hydrocarbons such as alka(e)nes are the major components of fossil fuels. Therefore, the biological production of these molecules in a sustainable fashion has gained tremendous attention in the past decade. Here, I will discuss the first successful overexpression and purification of a membrane-bound hydrocarbon-producing metalloenzyme (HPM) from bacterial cells. We establish that HPM is an oxygen and redox-dependent enzyme that converts fatty acids to hydrocarbons. We reconstitute the activity of HPM *in vitro* using several biological and chemical redox partners and identify the active metal in HPM. We also establish the substrate specificity and kinetic properties of the enzyme. Further, we provide a strategy to enhance the activity of the enzyme by a few hundred-fold. Our studies provide the framework to decipher the mechanism of HPM, which could serve as the fastest hydrocarbon-producing enzyme known to date.



References and Notes:

1. Iqbal, T.; Murugan, S.; and Das, D.* *To be submitted*
2. Iqbal, T. and Das, D.* *Biochemistry*, **2022**, *61*, 10, 909–921 [Featured as the Front Cover of the journal]
3. Iqbal, T.; Chakraborty, S.; Murugan S. and Das, D.* *Chemistry - An Asian Journal*, **2022,** *17*, e2022001 [Featured as the Front Cover of the journal]

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

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Debasis received his Ph.D. in Chemistry (Chemical Biology) from the University of Michigan, Ann Arbor, USA, in 2014. Followed by his postdoctoral work at MIT, USA, Debasis joined the Indian Institute of Science, Bangalore, as an assistant professor in 2019. His research area is interdisciplinary in nature, which has flavors of both Chemistry and Biology. His group focuses on the mechanistic understanding of various metalloenzymes and their applications. Employing various tools of chemistry, biochemistry, molecular biology, and microbiology, his group is exploring the function, kinetics, mechanism, and reaction intermediates of several poorly understood enzymes. The long-term goal of the work is to engineer and utilize these enzymes in green energy applications and therapeutics. He is a recipient of the Excellence of Research Award by the University of Michigan.

1. Iqbal, T. and **Das, D.*** Biochemical Investigation of Membrane-Bound Cytochrome b5 and Catalytic Domain of Cytochrome b5 Reductase from *Arabidopsis Thaliana- Accepted, **Biochemistry, 2022, 61, 10, 909–921*** [Featured as the **Front Cover** of the journal]

2. Ray, L. C.‡; **Das, D.**‡; Entova, S.; Lukose, V.; Lynch, A. J.; Imperiali, B.*; and Allen, K. N.* "Membrane Association of Monotopic Phosphoglycosyl Transferase Underpins Function." ***Nature Chem. Biol.*** **2018,** 14, 538-541. **(**‡ co-first author**)** [This article has been highlighted by **C&EN magazine**] [This article has been recommended by **F1000Prime** as being of special significance]

3. **Das, D**.; Kuzmic, P; and Imperiali, B.* "Analysis of a Dual Domain Phosphoglycosyl Transferase Reveals a Ping-Pong Mechanism with a Covalent Enzyme Intermediate." ***Proc. Natl. Acad. Sci. U.S.A.,*** **2017,** 114, 7019-7024. [This article has been recommended by **F1000Prime** as being of special significance]

4. Paul, B.;‡ **Das, D**.;‡ Ellington, B.;‡ and Marsh, E. N. G.* "Probing the Mechanism of Cyanobacterial Aldehyde Decarbonylase Using a Cyclopropyl Aldehyde" ***J. Am. Chem. Soc.,*** **2013,** 135, 5234-5237**. (**‡ co-first author**)**

5. **Das, D**.;‡ Eser, B. E.;‡ Han, J.; Sciore, A.; and Marsh, E. N. G.* "Oxygen-independent Decarbonylation of Aldehydes by Cyanobacterial Aldehyde Decarbonylase: a New Reaction of Di-iron Enzymes." ***Angew. Chem. Int. Ed.***, **2011**, *50*, 7148-7152. **(**‡ co-first author**)**

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
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Career Profile, significant awards/achievements and representative publications

Academic Records	1996; University of Calcutta (B.S.) 1998; University of Kalyani (M.S.) 2006; Indian Institute of Technology (IIT) Kanpur (Ph.D)	
Professional Career	2006~2008	Postdoc, Bar-Ilan University, Israel
	2008~2010	Postdoc, Drexel Nanotechnology Institute, USA
	2010~2015	Assistant Professor, IISER Kolkata
	2015~2019	Associate Professor, IISER Kolkata
	2016~2020	Founder Chair, Centre for Adv. Funct. Mater., IISER Kolkata
	2019~present	Professor, IISER Kolkata
Research Interests	1. Photovoltaics and optoelectronics with metal-halide perovskite nanostructures; 2. Electrochemical hydrogen fuel and CO_2 reduction; 3. Metal-air battery; 4. Photorechargeable battery	
Awards & Recognitions	2017 Emerging Investigator, J. Mater. Chem. A 2020 Life Fellow, Indian Chemical Society 2021 Editorial Advisory Board Member, ACS Applied Energy Materials 2021 Editor, Indian Journal of Chemistry 2021 SERB-STAR Award	

114 journal publications
1 conference proceeding
1 book chapter
1 Editorial
1 Educational Article

Accurate Molecular Dynamics Simulations with DFT

Nisanth N. Nair*
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Abstract:
Molecular dynamics (MD) simulations employing density functional theory (DFT) and plane waves are routinely carried out at the level of generalized gradient approximation (GGA). On the other hand, hybrid density functionals are more accurate and reliable than GGA functionals for predicting energetics and structural and dynamic properties. However, the computational cost for carrying out MD simulations using hybrid functionals and plane-wave basis sets is at least ***two orders*** of magnitude higher than that using GGA functionals. We propose a method to reduce the computational cost by at most ***two orders*** of magnitude. This technique has made it possible to study the mechanism and free-energetics of complex chemical reactions at the level of hybrid density functionals.

References and Notes:

1. Mandal, S.; Thakkur, V.; Nair, N. N. *J. Chem. Theory Comput.* **2021**, *17*, 2244-2255.

Bio-Sketch of Speaker

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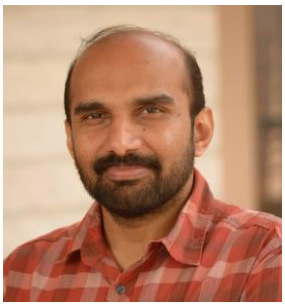

Education & Professional/Research Experience:

Professor	Nov 2018 – till now	Professor, Department of Chemistry, Indian Institute of Technology, Kanpur
Visiting Professor	May 2018- July 2018	Institute of Catalysis, Hokkaido University, Japan
Associate Professor	June 2014- Nov 2018	Department of Chemistry, Indian Institute of Technology, Kanpur
Assistant Professor	Dec. 2008 - June 2014	Department of Chemistry, Indian Institute of Technology, Kanpur
Post-Doctoral Fellow	Jan. 2005 – Dec. 2008	Ruhr University, Bochum, Germany
Ph. D.	Oct. 2001 – Dec. 2004	University of Hannover, Germany
M. Sc. Chemistry	July 1999 – June 2001	Indian Institute of Technology, Madras, Chennai, India

Peer Recognition/Awards:

Young Scientist Medal, Indian National Science Academy (INSA), New Delhi	2013
Young Associate of the Indian Academy of Sciences (IAS), Bangalore	2012-2015
P K Kelkar Young Faculty Research Fellow, IIT Kanpur	2012-2015
Excellence in Teaching Award, IIT Kanpur	2019
Distinguished Lectureship Award, Chemical Society of Japan	2018
Member of the Scientific Advisory Board of Quantumzyme LLP	2020-2022
Visiting Professor, Institute of Catalysis, Hokkaido University, Japan	2018
Member of Expert Committee, MATRICS, SERB	2021-22

Five Selected Publications:

1. S. Mandal, V. Thakkur, Nisanth N. Nair, Achieving an Order of Magnitude Speedup in Hybrid Functional- and Plane-Wave-Based Ab Initio Molecular Dynamics: Applications to Proton-Transfer Reactions in Enzymes and in Solution, J. Chem. Theory Comput. **17**, 2244 (2021).

2. Abhinav Gupta, Shivani Verma, Ramsha Javed, Suraj Sudhakar, Saurabh Srivastava, Nisanth N. Nair, *Exploration of high dimensional free energy landscapes by a combination of temperature-accelerated sliced sampling and parallel biasing*, J. Comput. Chem. 43, 1186 (2022).

3. Shalini Awasthi and Nisanth N. Nair, *Exploring high dimensional free energy landscapes: Temperature accelerated sliced sampling*, J. Chem. Phys. **146,** 094108 (2017).

4. Sudhir K Sahoo and Nisanth N. Nair, *Interfacing the Core-Shell or the Drude Polarizable Force Field With Car-Parrinello Molecular Dynamics for QM/MM Simulations*, Frontiers in Chemistry 6, 275 (2018).

5. C. K. Das, Nisanth N. Nair, *Elucidating the Molecular Basis of Avibactam Mediated Inhibition of Class A Beta-Lactamases*, Chem. Eur. J. **26**, 9639-9651 (2020).

Effects of noise on cellular processes and signaling pathways

Rati Sharma*

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Abstract:

All cellular processes are characterized by noise because of the microscopic nature of the system. This noise, generally, can be categorized into two components - intrinsic and extrinsic. Intrinsic noise is a result of the inherent randomness in the system in terms of the stochasticity in the number of molecules undergoing a reaction at a particular time. Extrinsic noise, on the other hand, is the randomness that is caused by factors external to the system of interest.

In this talk, I will discuss the role of noise in three specific biological processes viz. (i) the effects of extrinsic noise on mRNA translation process [1]; (ii) bistability in the heat shock response pathway due to the presence of intrinsic noise [2] and (iii) effects of non-Markovian (colored) noise on the virus-immune response pathway, with particular consideration for the SARS-CoV-2 virus [3,4].

References:

1. Extrinsic noise effects on ribosomal traffic during the translation process. Rati Sharma*. J. Stat. Mech: Theory Exp. 053504 (2022).

2. Transcription factors and chaperone proteins play a role in launching a faster response to heat stress and aggregation. Sushmita Pal and Rati Sharma*. Comput. Biol. and Chem. 93, 107534 (2021).

3. A near analytic solution of a stochastic immune response model considering variability in virus and T cell dynamics. Abhilasha Batra and Rati Sharma*. J. Chem. Phys. 154, 195104 (2021).

4. Persistent correlation in cellular noise determines longevity of viral infections. Abhilasha Batra, Shoubhik Chandan Banerjee and Rati Sharma*. Under review.

Bio-Sketch of Speaker

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Dr. Rati Sharma is an Assistant Professor in the Dept. of Chemistry at Indian Institute of Science Education and Research (IISER) Bhopal. She graduated in Chemistry from Stella Maris College, Madras University in 2007. Following this, she joined the Integrated PhD program of the Division of Chemical Sciences at Indian Institute of Science, Bangalore, where she completed her MS and PhD in 2013 under the guidance of Prof. Binny J. Cherayil. Her PhD thesis primarily focussed on questions in theoretical biophysics and polymer physics. She then pursued postdoctoral research at the Dept. of Biophysics, Johns Hopkins University, USA from 2013-2016 and at the Dept. of Physics, Harvard University, USA from 2016 to 2018. Her postdoctoral research training encompassed a variety of topics in systems biology, where she gained experience in Monte Carlo simulations, machine learning, microfluidics, stress response microscopic studies and image analysis.

She moved back to India in 2019 where she has steadily established her group. She has received grants from both DST-SERB and DBT since she joined IISER Bhopal. She has recently also been awarded the SERB-POWER grant. Her current research interests focus on computational and experimental biophysics, ranging from topics such as stress response dynamics studies in *C. elegans*, modeling of immune response dynamics, machine learning applications to biomedical research to computational studies of signaling pathways, to name a few.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
…Anticipating Tomorrow's Science through Collaborative Ventures

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Buddhadeb graduated (2003) with M.Sc. in Organic Chemistry from Visva-Bharati University (Santiniketan) and earned Ph.D. degree in Synthetic Organic Chemistry from the University of Kalyani (2009), West Bengal. In 2009, he accepted a postdoctoral research associateship from the University of Illinois at Chicago, USA in the group of Professor Vladimir Gevorgyan. Spending two years at Chicago, he then moved to the Michigan State University, Michigan, USA for his next postdoctoral research program in the laboratories of Professor Milton R. Smith III. Group (2011-July 2014). In August 2014, he started his independent career at Centre of Biomedical Research (CBMR) Lucknow. Since 2019, he is serving in the same institute as Associate Professor, Chemistry. His research interest includes design and synthesis of new catalytic systems employing various noncovalent interactions for the C–H bond activation/borylation chemistry and synthesis of medicinally important high-valued N-heterocyclic molecules via metal-nitrene/carbene chemistry. Buddhadeb is a recipient of Thieme Chemistry Journal Award (2017), DST-Young Scientist Award (2015), Ramanujan Fellowship (2014) and SERB-STAR Award (2019).

Selected Publications:

Formal Ir-Catalyzed Ligand-Enabled Ortho- and Meta-Borylation of Aromatic Aldehydes via in Situ Generated Imines. Bisht, R.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2016**, *138*, 84-87.

Non-Covalent Interactions in Ir-Catalyzed C–H Activation: L-Shaped Ligand for Para-Selective Borylation of Aromatic Esters. Hoque, E.; Bisht, R.; Haldar, C.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2017**, *139*, 7745-7748.

Ir-Catalyzed Intramolecular Transannulation/C(sp^2)–H Amination of 1,2,3,4-Tetrazoles by Electrocyclization. Das, S. K.; Roy, S.; Khatua, H.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2018**, *140*, 8429-8433.

Remarkably Efficient Iridium Catalysts for Directed C(sp2)–H and C(sp^3)–H Borylation of Diverse Classes of Substrates. Hoque, E.; Hassan, M. M. M.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2021**, *143*, 5022–5037.

Meta Selective C–H Borylation of Sterically Biased and Unbiased Substrates Directed by Electrostatic Interaction. Chaturvedi, J.; Haldar, C.; Bisht, R.; Pandey, G.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2021**, *143*, 7604-7611.

Remarkably Efficient Iridium Catalysts for Directed C(sp^2)–H and C(sp3)–H Borylation of Diverse Classes of Substrates. Hoque, E.; Hassan, M. M. M.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2021**, *143*, 5022–5037.

Road Map for the Construction of High-Valued N-Heterocycles via Denitrogenative Annulation. Roy, S.; Das, S. K.; Khatua, H.; Das, S.; Chattopadhyay, B. *Acc. Chem. Res.* **2021**, *54*, 4395–4409.

Metal-Catalysed C–H Bond Activation and Borylation. Bisht, R.; Haldar, C.; Hassan, M. M. M.; Hoque, E. M.; Chaturvedi, J.; Chattopadhyay, B. *Chem. Soc. Rev.* **2022**, *51*, 5042-5100.

Probing chemical space tolerance of DNA polymerases in real time and 3D

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Abstract:
DNA and RNA polymerases and nucleotide transferases are highly useful in introducing functionalities that aid in the structural and functional analysis of nucleic acids. Though it is difficult to predict the substrate tolerance of these enzymes, nucleotides modified at the base serve as good substrates for enzymatic incorporation. However, the molecular basis by which these enzymes incorporate and process functionalized nucleotide substrates is not yet fully understood. In this context, biochemical and X-ray techniques have been used to study the mechanism of incorporation of few of the modified nucleotides.[1] The results from these studies are indicative, and hence, a detailed understanding of the chemical space tolerance of the polymerases is required. For a decade now, we have been interested in developing microenvironment-sensitive fluorescent nucleosides analogs that help in probing the structure and ligand binding properties of therapeutic nucleic acid motifs.[2-6] The nucleoside/nucleotide analogs are built by attaching heterocycles onto the purine and pyrimidine bases, and some of these are good substrates for enzymes. In this presentation, I will describe the development of a novel platform to probe the chemical space tolerance and the mechanism of incorporation of DNA polymerases by fluorescence and X-ray crystallography using our environment-sensitive nucleotide probes.[7] Here, the fluorescent nucleotide substrates itself serve as probes to study the activity of DNA polymerases.

References:

1. Hottin, A.; Marx, A. *Acc. Chem. Res.* **2016**, *49*, 418−427.
2. Nuthanakanti, A.; Boerneke, M. A.; Hermann, T.; Srivatsan S. G. *Angew. Chem. Int. Ed.* **2017**, *56*, 2640–2644.
3. Manna, S.; Sarkar, D.; Srivatsan, S. G. *J. Am. Chem. Soc.* **2018**, *140*, 12622–12633.
4. Ashok, N.; Ishtiyaq, A.; Saddam, Y. K.; Kayarat, S.; Srivatsan, S. G. *Nucl. Acid. Res.* **2019**, *47*, 6059–6072.
5. Manna, S.; Srivatsan, S. G. *Org. Lett.* **2019**, *21*, 4646−4650.
6. George, J. T.; Srivatsan, S. G. *Chem. Commun.* **2020**, 56, 12319−12322.
7. Ghosh, P.; Kropp, H. M.; Betz, K.; Ludmann, S.; Diederichs, K.; Marx, A.; Srivatsan S. G. *J. Am. Chem. Soc.* **2022**, *144*, 10556–10569.

Bio-Sketch of Speaker

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S. G. Srivatsan received his master's degree in Chemistry from Indian Institute of Technology, Madras in 1995 and Ph. D. in Bioorganic Chemistry from Indian Institute of Technology, Kanpur in 2003 under the supervision of Prof. Sandeep Verma. He was an Alexander von Humboldt postdoctoral fellow with Prof. Michael Famulok at University of Bonn, Germany, where he developed catalytic RNAs and pharmacophores that target protein-RNA complexes and their enzyme activity. Subsequently, he joined Prof. Yitzhak Tor group as a postdoctoral fellow in University of California, San Diego. He joined Indian Institute of Science Education and Research (IISER), Pune in November 2008. He is currently a Professor and Wellcome Trust-DBT India Alliance Senior Fellow. He received the CDRI AWARDS–2019 for Excellence in Drug Research, Chemical Research Society of India Bronze medal (2020), National Prize for Research on Chemistry of Peptides and Nucleic Acids 2020 (sponsored by Professor CNR Rao Education Foundation) and Sun Pharma Research Award 2020. He also serves as an Editorial Advisory Board member of ACS Bioconjugate Chemistry. His research interests lie in the area of nucleic acid chemistry and biophysics, particularly in the development of nucleoside probes for studying nucleic acid structure and function, nucleoside-based self-assemblies, and nucleic acid labeling and imaging tools.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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A donor-acceptor cyclopropane with spiropyran-like behavior and catalyst-free water activation emerging from NHC vs. CAAC comparison

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Indian Institute of Science Education and Research Kolkata
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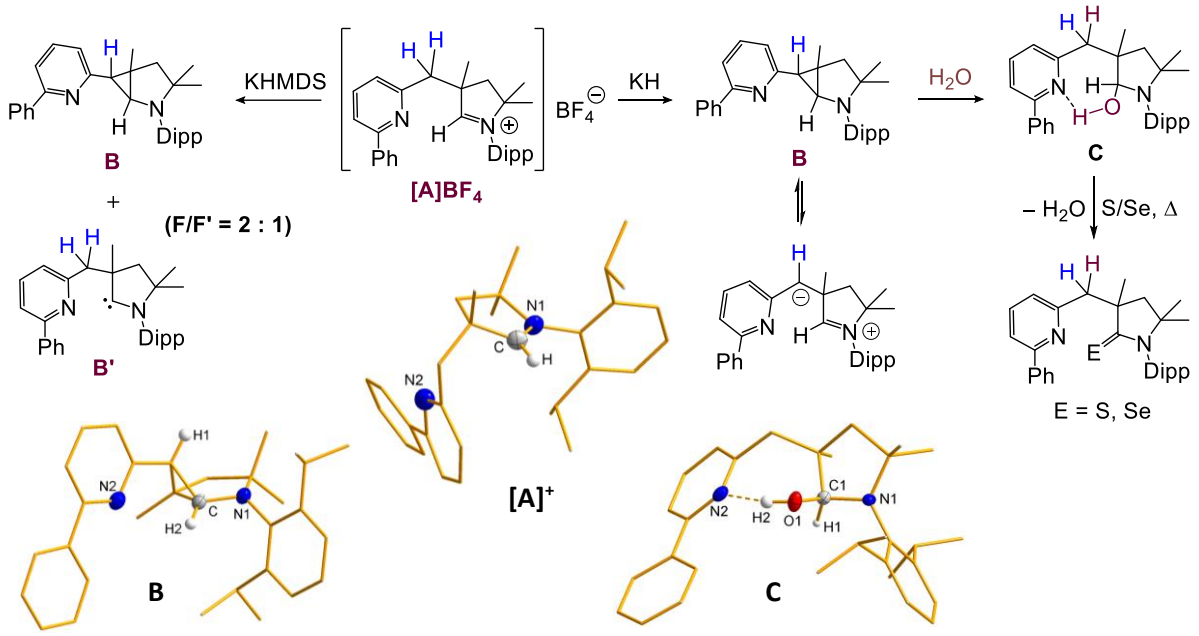
Abstract:
An attempt to develop a picolyl-tethered CAAC [cyclic alkyl(amino) carbene] reveals many interesting chemistries in contrast to its NHC analogue. The divergence between the 2-*H*-imidazolium and 2-*H*-pyrolinium precursors results from their electrophilicity difference and the disparity in acidity. In case of the later, the picolyl protons appear to be more vulnerable towards deprotonation leading to many surprises as summarized below. The deprotonation of **[A]BF$_4$** is base-specific showing a clear distinction between KH and KHMDS. KH deprotonates **[A]BF$_4$** at the picolyl position giving the donor-acceptor (DA) cyclopropane derivative **B** which shows a thermal-driven spiropyran like behavior and is readily ring-opened by H_2O to give **C**. Deprotonation by more soluble KHMDS interestingly gives a 2:1 mixture of **B** and another species which can be spectroscopically assigned as the desired CAAC species **B'**. The later undergoes picolyl C-H activation upon heating to convert into **B**. The secondary alcohol **C** can be dehydrated in the presence of sulfur or selenium to give their corresponding carbene adducts.



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1. Chu, J.; Munz, D.; Jazzar, R.; Melaimi, M.; Bertrand, G., *J. Am. Chem. Soc.* **2016**, *138*, 7884.
2. Kang, Q-K.; Wang, L.; Liu, Q-J.; Li, J-F.; Tang, Y. *J. Am. Chem. Soc.* **2015**, *137*, 14594.
3. Kortekaas, L.; Browne, W. R. *Chem. Soc. Rev.* **2019**, *48*, 3406.

Bio-Sketch of Speaker

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Career Profile:

Assistant Professor:	June 2019-	IISER Kolkata
Assistant Professor:	March 2018-May 2019	IIT Kharagpur
Alexander von Humboldt Postdoc Fellow:	March 2015-February 2018	RWTH Aachen University, Germany
Postdoc	May 2013-December 2014	Argonne National Lab, USA
PhD	August 2007-December 2012	Iowa State University, USA

Significant awards:

Ramanujan Fellowship, SERB India, 2018
Alexander von Humboldt Postdoc Fellowship, AvH Foundation, Germany, 2014
Frank J. Moore and Thoreen Beth Moore Fellowship, Iowa State University, USA, 2011
Outstanding mentor award, US-DOE, Office of Science, Ames Laboratory, USA 2011
Chevron Phillips Fellowship, Iowa State University, USA, 2010

Representative publications:

1. Baguli, S.; Mondal, S.; Mandal, C.; Goswami, S.; Mukherjee, D.* "Cyclopentadienyl and Carbene Complexes of the Alkaline Earths in the Light of Periodic Trends" *Chem. Asian. J.* **2021**, DOI: *10.1002/asia.202100962*.
2. Mukherjee, D.*; Schuhknecht, D.; Okuda, J.* "Hydrido complexes of calcium: a new family of molecular alkaline earth metal compounds." *Angew. Chem. Int. Ed.* **2018**, *57*, 9590-9602.
3. Mukherjee, D.*; Okuda, J.* "A monoanionic NNNN-type macrocyclic ligand for electropositive metal centers." *Chem. Commun.* **2018**, *54*, 2701-2714.
4. Mukherjee, D.; Höllerhage, T.; Leich, V.; Spaniol, T.P.; Englert, U.; Maron, L.; Okuda, J.* "The nature of the heavy alkaline earth metal-hydrogen bond: synthesis, structure, and reactivity of a cationic strontium hydride cluster." *J. Am. Chem. Soc.* **2018**, *140*, 3403-3411.
5. Mukherjee, D.*; Okuda, J.* "Molecular magnesium hydrides." *Angew. Chem. Int. Ed.* **2018**, *57*, 1458-1473.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
…Anticipating Tomorrow's Science through Collaborative Ventures

Nitin T. Patil

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Academic Qualifications:

- Ph.D. (**1997-2002**): University of Pune, India
- M.Sc. (**1995-1997**): North Maharashtra University, Jalgaon, India
- B.Sc. (**1992-1995**): North Maharashtra University, Jalgaon, India

Professional Experience:

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

Dr. Patil's broad research interests include the development of metal-, organo- and organo/metal-catalyzed enantioselective methods as well as total synthesis of natural products. He has been the recipient of the SERB Distinguished Investigator Award, CRSI Bronze Medal, INSA Young Scientist Medal, Alkyl Amines – ICT Foundation Day Young Scientist Award and Avra Young Scientist Award. He has also served as "Young Associate" of the Indian Academy of Sciences, Bangalore during 2010-2013. Recently, he was elected as a Fellow of the Indian National Science Academy (FNA), a Fellow of The National Academy of Sciences (FNASc), a Fellow of Maharashtra Academy of Sciences (FMASc) and a fellow of The Royal Society of Chemistry (FRSC).

Targeting IMPDHs to overcome resistance in Bacteria: A case study with *Helicobacter pylori*

Sivapriya Kirubakaran *
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Abstract:

Developing nations like India are home to a wide range of tropical diseases, few of which are found to directly cause long-term effects including cancer. Inosine-5'-monophosphate dehydrogenase the oxidoreductase enzyme that kicks off a series of reactions constituting the *de novo* purine biosynthesis pathway, has been identified as a potential drug target to treat several disease conditions. The reaction catalyzed by IMPDH, which converts inosine-5'-monophosphate to xanthosine-5'-monophosphate with the help of NAD^+, is a precursor for DNA and RNA synthesis using guanine nucleotides, hence promoting growth and proliferation of the pathogen in the host[1]. *Helicobacter pylori*, one among such infectious pathogens, is a causative agent for several acute and chronic gastrointestinal ulcers and gastric cancer, as a result of its colonization of the gastric mucosa. Our lab focuses on studying Hp IMPDH along with other IMPDHs from Leishmania, Mycobacterium with help of small molecules to study the mechanism of this enzyme when its mutated as a futuristic study to tackle AMR. How the interdisciplinary research pushes us in developing a potent molecule from organic chemistry lab bench to preclinical trials will be discussed in the presentation.

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2. Kirubakaran, S.; Gorla, S. K.; Sharling, L. *et al*, *Bioorg. Med. Chem. Lett.*, **2012**, 22, 1985-8.
3. Juvale, K.; Shaik, A.; Kirubakaran, S., *Med. Chem. Commun.*, **2019**, *10*, 1290-130.
4. Juvale, K.; Purushothaman, G.; Singh, V.; Shaik, A.; Ravi, S.; Thiruvenkatam, V.; Kirubakaran, S. Identification of selective inhibitors of *Helicobacter pylori* IMPDH as a targeted therapy for the infection. *Sci. Rep.*, **2019**, *9* (1), 1-10.
5. Jangra, S.; Purushothaman, G.; Juvale, K.; Ravi, S.; Menon, A.; Thiruvenkatam, V.; Kirubakaran, S. Synthesis and In Vitro Enzymatic Studies of New 3-Aryldiazenyl Indoles as Promising *Helicobacter pylori* IMPDH Inhibitors. *Curr Top Med Chem*. **2019**, *19* (5), 376-382.
6. Dilip, H.; Purushothaman, G.; Sharma, G.; Menon, A.; Thiruvenkatam, V.; Kirubakaran, S. Mutants of *Helicobacter pylori* IMPDH: kinetics and in silico studies to determine the structural and functional role of key amino acids. *Chem. Asian J.*, **2022**, *17* (9), e202200125.

Bio-Sketch of Speaker

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Dr. Sivapriya Kirubakaran did her Ph.D. (Organic chemistry) from Indian Institute of Science, Bangalore under the supervision of Prof. S. Chandrasekaran, and did her Postdoctoral Fellowships from Harvard Medical School and Whitehead Institute, MIT. She is an associate professor and Kankuben Bakshiram Gelot Chair in chemistry at Indian Institute of Technology, Gandhinagar. She is the current Dean of students at IITGN. She has co-authored about 42 publications, 1 book chapter and have 8 US and 14 Indian patents to her credit. She is also a recipient of the prestigious DST Ramanujan Fellowship (2013-2018). Her current areas of interest include targeted drug discovery and medicinal chemistry. Her lab focuses on studying mechanistic pathways of DDR kinases using small molecules to develop novel therapeutics as well exploring *Helicobacter pylori* survival pathways for developing drugs against the infection. Her long-term goal would be to make affordable medicines for cancer.

Synthesis of New Green High Energy Density Materials with Fine-tuned Properties

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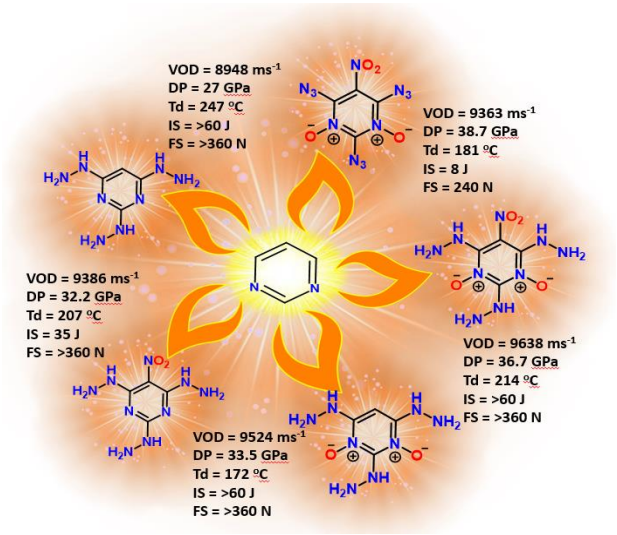
Abstract:
The history of energetic materials is demonstrating that the synthesis and development of green high-energy density material and energetic oxidizers is always a challenging problem for energetic material chemist.[1] Taking this into the consideration, here I am going to present the synthesis and use of some known explosives, which are ammonium nitrate (AN), pentaerythritol tetranitrate (PETN), trinitrotoluene (TNT) and hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX),3 etc. With this, I will present newly synthesized green high energy density materials, their energetic properties and where these will stand with the existing molecules such as TNT, RDX, HMX, FOX-7 and CL-20.[2]

Figure:



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2. a) Zhang, J.; Mitchell, L. A.; Parrish, D. A.; Shreeve, J. M. *J. Am. Chem. Soc*. **2015**, *137*, 10532−10535; b) Dharavath, S.; Mitchell, L. A.; Parrish, D. A.; Shreeve, J. M.; *Chem. Commun.*, **2016**, *52*, 7668-7671.
3. a) Abhishek K. Y.; Parasar K.; Vikas D. G.; Srinivas D. *Asian J. Org. Chem.*, **2022,** https://doi.org/10.1002/ajoc.202100779. b) Abhishek K. Y.; Vikas G. D.; Srinivas D, *Mater. Chem. Front.*, **2021,** *5*, 8352-8360.

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

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Experience:

1. Indian Institute of technology, Kanpur, India 2019-till
Assistant professor, Department of Chemistry

2. McMaster University, Hamilton, Canada
Postdoctoral fellow in the group of Prof. Jakob Magolan, **2017-2009**

3. University of Idaho, Moscow, USA-Department of Chemistry
Postdoctoral fellow in the group of Prof. J. M. Shreeve, **2015-2017**

4. University of Hyderabad, Hyderabad, India - School of Chemistry
Postdoctoral fellow in the group of Dr. K. Muralidharan, **2015**

Education:

1. **University of Hyderabad, Hyderabad, India - ACRHEM**
Ph.D. (Heterocyclic Chemistry/Energetic Materials Chemistry), **August 2010–December 2014**, University of Hyderabad, Hyderabad, India. **"Design and Synthesis of Nitrogen-rich Heterocyclic Compounds and Salts as Energetic Materials."**

2. M.Sc. (Organic Chemistry), **2007-2009**, Osmania University, Hyderabad, India.

3. B.Sc. (Chemistry, Botany and Zoology), **2003-2006**, Osmania University, Hyderabad, India.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
…Anticipating Tomorrow's Science through Collaborative Ventures

Subhash Chandra Ghosh

Principal Scientist

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Subhash Chandra Ghosh was born (1976) in Midnapore, West Bengal, India. He received his B.Sc (Midnapore College) and M.Sc. degree from Vidyasagar University in 1997 and 1999 respectively. He worked with Prof. Amit Basak at IIT-Kharagpur and received his Ph.D. degree in 2006. In April 2006 he joined as a postdoctoral fellow at POSTECH, South Korea with Professor Sung Kee Chung where he worked on the total synthesis of KRN 7000 and it's all 8 stereoisomers and on inositol-based molecular transporter. In November 2008 he moved from POSTECH to NTU, Singapore, and joined as a research fellow with Prof. Hong Soon Hyeok and started working on Ru catalyzed direct amide synthesis. Later, in October 2010 he moved to ICES, A*STAR, Singapore as a Scientist I and worked on GSK funded project on a new route on amide synthesis. Since December 2012, he is working as a scientist at CSIR-CSMCRI, India to pursue his professional research career.

Representative publications

- *Copper(II) mediated ortho C–H alkoxylation of aromatic amines using organic peroxides: efficient synthesis of hindered ethers* S. Sarkar, T. Sahoo, C. Sen, S. C. Ghosh *Chem. Commun.* **2021,** *57*, 8949–8952
- *C–H Amidation and Amination of Arenes and Heteroarenes with Amide and Amine using Cu-MnO as a Reusable Catalyst under Mild Conditions* H. Singh, C. Sen, E. Suresh, A. B. Panda, S. C. Ghosh *J. Org. Chem.* **2021**, *86, 3261–3275*
- *Room-Temperature Synthesis of Isoindolone Spirosuccinimides: Merger of Visible-Light Photocatalysis and Cobalt-Catalyzed C–H Activation* C. Sen, B. Sarvaiya, S. Sarkar, S. C. Ghosh *J. Org. Chem*. **2020**, *85*, 15287–15304
- *"Visible Light Promoted Photocatalytic C-5 Carboxylation of 8-Amino Quinoline Amides and Sulfonamides via a Single Electron Transfer Pathway" C.* Sen, T. Sahoo, H. Singh, E. Suresh, S. C. Ghosh *J. Org. Chem.* **2019**, *84*, 9869−9896

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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Swarm Intelligence Guided Global Minima Search on Complex Potential Energy Surfaces

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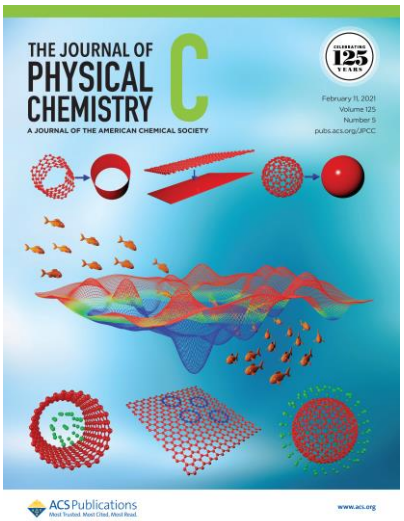
Abstract:
One of the current day challenges in theoretical chemistry is the optimization of complex chemical systems with large number of degrees of freedom.[1] The potential energy surfaces associated with the non-covalent interactions involving nanostructures and atomic or molecular clusters are often rugged with a large number of local minima hindering tracking down of the global minima. Global optimization techniques are indispensable to attain the global minima configurations of such complex systems.[1,2] In this talk, I shall describe some of our recently explored optimal theoretical design strategies for investigating the binding of some Lennard-Jones clusters with nanostructures by amalgamating the continuum and discrete formulations of intermolecular interactions with particle swarm optimization (PSO), one of the swarm intelligence techniques falling under the general ambit of artificial intelligence.[3-9] I shall also exemplify the hierarchy of empirical potentials by depicting them on the various rungs of the Jacob's ladder equivalent of density functional theory for the intermolecular force fields.[10] The intermolecular force fields thus-developed could be employed in dynamical simulations and the putative global minima geometries obtained from our methodology could be excellent starting points for first-principles calculations.



References and Notes:

1. Wales, D. J. *et al. Science* **1999**, *285*, 1368-1372.
2. Hernandez-Rojas, J. *et al. J. Phys. Chem. C* **2012**, *116*, 17019-17028.
3. Hilder, T. A. *et al. J. Phys. A: Math.Theor.* **2007**, *40*, 3851-3868.
4. Swathi, R. S. and co-workers *J. Phys. Chem. C* **2021**, *125*, 2811–2823 [invited perspective].
5. Swathi, R. S. and co-workers *Phys. Chem. Chem. Phys.* **2020**, *22*, 20693-20703.
6. Swathi, R. S. and co-workers *Eur. Phys. J. D.* **2021**, *75*, 1-14 [invited article; special issue on confinement effects].
7. Chris, J.; Swathi, R. S. *Phys. Chem. Chem. Phys.* **2022**, *24*, 2554-2566.
8. Chris, J.; Megha, R.; Swathi, R. S. *Chem.: Asian J.* **2022** (in press).
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10. Swathi, R. S. and co-workers *WIREs Comput. Mol. Sci.* **2022,** *12*, e1599.

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

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R. S. Swathi obtained an integrated B. Sc. Ed degree from Regional Institute of Education, Mysore and an M. Sc. Degree in Chemistry from Indian Institute of Technology, Guwahati. Subsequently, she pursued PhD in theoretical chemistry from Indian Institute of Science, Bangalore working under the supervision of Prof. K. L. Sebastian. Since 2010, Swathi has been working as a faculty member at the School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram and is currently an Associate Professor there. Her multiscale modelling and computation group employs analytical and computational approaches for modeling interesting phenomena involving carbon-based and metal-based nanostructures. Swathi is a recipient of the Young Scientist Awards from Indian National Science Academy, National Academy of Sciences, Kerala State Council for Science, Technology and Environment, and Distinguished Lectureship Award from the Chemical Society of Japan. Swathi was also a young associate of the Indian Academy of Sciences, Bangalore. Swathi is a recipient of the A V Rama Rao Foundation Prize in Chemistry awarded by the JNCASR, Bangalore for the year 2020.

Publications:

1. Chris, J..; Megha, R.; Swathi, R. S. *Chem.: Asian J.* **2022** (in press).
2. Anto, J.; Swathi, R. S. *J. Phys. Chem. A* **2022,** *126*, 3472-3485.
3. Anto, J.; Chris, J.; Ajay, M.; Megha, R.; Swathi, R. S. *WIREs Comput. Mol. Sci.* **2022,** *12*, e1599.
4. Chris, J.; Swathi, R. S. *Phys. Chem. Chem. Phys.* **2022**, *24*, 2554-2566.
5. Ajay, M.; Anto, J.; Megha, R.; Chris, J.; Swathi, R. S. *Phys. Chem. Chem. Phys.* **2021**, *23*, 27031-27041.
6. Chris, J.; Owais, C. H.; Anto, J.; Swathi, R. S. *J. Phys. Chem. C* **2021**, *125*, 2811–2823 [invited perspective].
7. Anvy, K.; Naidu, G. N.; Swathi, R. S. *J. Phys. Chem. C* **2020**, *124*, 13858–13871.
8. Rama, D.; Chris, J.; Swathi, R. S. *J. Phys. Chem. A* **2019**, *123*, 7499-7506.
9. Anto, J.; Swathi, R. S. *J. Phys. Chem. C.* **2019**, *123*, 10544-10556.
10. Mahroof, K.; Owais, C. H.; Roy, D. S. P.; Swathi, R. S. *ACS Omega* **2018**, *3*, 7542-7554.

Genetically encodable fluorescent RNA sensors for metal ions, small molecule and macromolecule detection

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Department of Chemistry and Biology
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Abstract:
Nucleic acid sensing holds great potential in disease diagnosis, gene expression profiling and personalized therapeutic approaches. Several nucleic acid based sensors for the detection of small molecule as well as macromolecules such as DNA/RNA has been reported in literature. Most of the nucleic acid based sensors require chemical labelling with fluorophores and thus are not genetically encodable to be expressed in cells. We utilized fluorescent light-up aptamer based sensors for small molecule and nucleic acid sensing. Fluorescent light-up aptamers such as widely used Spinach aptamers has been shown to activate the fluorescence of otherwise non-fluorescent small-molecule DFHBI (3,5-difluoro-4-hydroxybenzylidene imidazolidinone)[1]. Using a miniature variant of spinach aptamer, termed as baby spinach, we have demonstrated a surprisingly simple, cost effective and label free baby spinach based minimalistic sensor (BSMS) for fluorescent detection of nucleic acids including miRNAs[2]. In addition, we have demonstrated that fluorescent light-up aptamer acts as a reversible conformational switch in the presence of small molecules/metal ions. This will provide not only the control on the aptamer system that is needed for on-demand functionality of the aptamer but will also be used to detect small molecules/metal ions in vitro as well in cells by encoding the sensor as a gene product.

References and Notes:

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Dr. Ashwani Sharma completed his PhD in 2011 from National Chemical Laboratory (NCL), Pune. He did his post-doctoral studies from University of Utah and Markey Cancer Centre, University of Kentucky, USA from 2011–2015. After coming back to India, he joined as DST young scientist in Indian Institute of Chemical Technology (IICT), Hyderabad for a short span of one year. He joined IISER Tirupati as an Assistant Professor in 2017. His area of interest is RNA biology. His lab work on RNA nanotechnology for targeted drug delivery, developing RNA aptamers, ribozymes and utilizing them in the detection of small molecules as well as macromolecules, RNA engineering for efficient gene editing, and to understand the role of various non-coding RNAs in the cell.

Ashwani Kumar Tiwari

Professor

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Ashwani K. Tiwari received his Ph.D. in 2007 from the Indian Institute of Technology Kanpur under the supervision of Prof. N. Sathyamurthy. During the period from May 2007 to April 2008, he was a postdoctoral researcher with Prof. Niels E. Henriksen at the Technical University of Denmark. From May 2008 to April 2010, he was a postdoctoral fellow with Prof. Bret Jackson at the University of Massachusetts, Amherst. He joined the Indian Institute of Science Education and Research Kolkata as an assistant professor in October 2010, and now he is a professor at the same institute. His research interests involve the dynamics of laser–molecule and molecule–metal surface interactions. Recently, he received the Chemical Research Society of India (CRSI) Bronze Medal and was elected as fellow of Royal Society of Chemistry.

Recent Publications:

1. Mode Selective Chemistry for the Dissociation of Methane on Efficient Ni/Pt-Bimetallic Alloy Catalysts; S. Roy and **A. K. Tiwari** ***Phys. Chem. Chem. Phys.*****, XX,** XX (2022).
2. Oxygen-Induced Dissociation of a Single Water Molecule in Confined 2-D Layers: A Semiempirical study; M. Majumder and **A. K. Tiwari** ***Chem. Phys. Chem,*** **XX,** XX (2022).
3. Attosecond coupled electron-nuclear dynamics of H_2 molecule under intense laser fields; G. Pandey and **A. K. Tiwari** ***Eur. Phys. J. D,*** **76,** 75 (2022).
4. Schematic Design of Metal-Free NHC-Mediated Sequestering and Complete Conversion of SO_2 to Thiocarbonyl S-Oxide Derivatives at Room Temperature ; R. Logdi, A. Bag and **A. K. Tiwari** ***J. Phys. Chem. A.*****, 126,** 221-229 (2022).
5. Effcient Water-Gas Shift Catalysts for H_2O and CO Dissociation using Cu-Ni Step Alloy Surfaces; S. Roy and **A. K. Tiwari** ***J. Phys. Chem. C.*****, 125,** 13819-13835 (2021).
6. Controlling the ultrafast dynamics of HD^+ by the carrier-envelope phases of an ultrashort laser pulse: A quasi-classical dynamics study; G. Pandey, D. Dey and **A. K. Tiwari** ***J. Phys. Chem. A.*****, 124,** 9710-9720 (2020)

Emergence of Cooperativity from Multivalent Interactions

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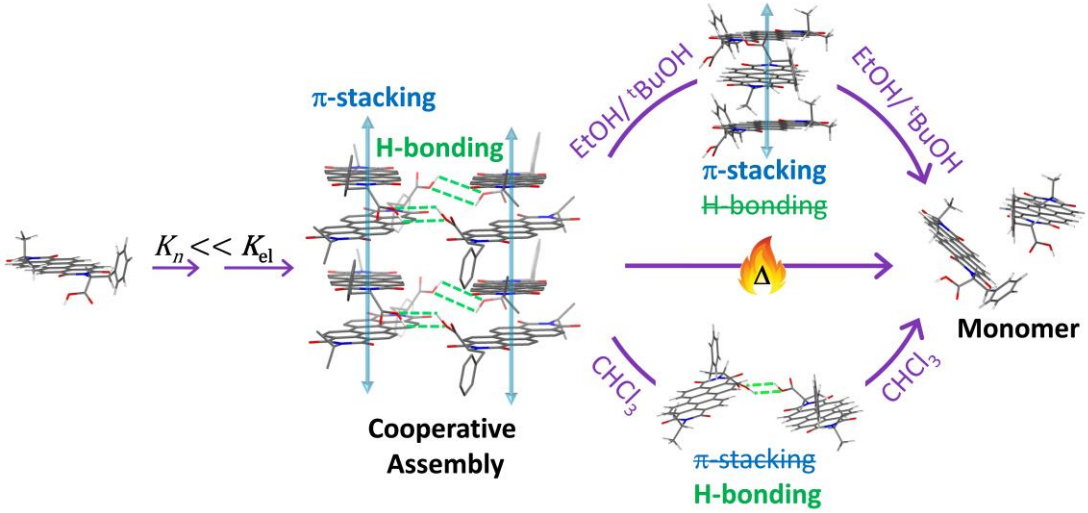
Abstract:
Self-assembly of small molecules is of great significance in material science, systems chemistry and synthetic biology. Last decade has seen several breakthroughs in the area of programmable self-assembly, which underscores the importance of cooperative interactions in achieving control over molecular self-assembly. Emerging from a complex interplay of short and long-range noncovalent interactions, achieving cooperativity has largely relied on empirical knowledge. Its development as a rational design tool in molecular self-assembly requires a detailed characterization of the underlying interactions, which has been a challenge. This talk will address two important questions pertaining to cooperativity in molecular self-assembly: its molecular origin and characterization. Using one- and two-dimensional magic-angle-spinning (MAS) solid-state NMR spectroscopy, key structure-directing interactions were identified in cooperatively bound aggregates. Analyses of ^{1}H-^{13}C cross-polarization heteronuclear correlation (CP-HETCOR) and 1H-1H double-quantum single-quantum (DQ-SQ) correlation spectra allow the identification of through-space proximities in the assembled state. Emergence of cooperativity from synergistic interaction between a stronger π-stacking and a weaker interstack hydrogen-bonding is also elucidated. Finally, a combination of optical absorption, circular dichroism and high-resolution MAS NMR spectroscopy reveals the anomalous nature of solvent-induced disassembly. Our results highlight the disparity between two well-established approaches of characterizing cooperativity. Finally, our approach underscores the importance of bridging the gap between solution-phase characterization techniques and solid-state structure elucidation, the applicability of which extends beyond supramolecular chemistry to other disordered material systems.



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2. Rest, C.; Kandanelli, R.; Fernandez, G. *Chem. Soc. Rev.* **2015**, *44*, 2543−2572.
3. Samanta, S.; Raval, P.; Reddy, G. M. N.; Chaudhuri, D. *ACS Centr. Sci.* **2021**, *7*, 1391-1399.

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

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Bio-Sketch of Speaker

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Research Interests

Development of efficient routes for the syntheses of carbene stabilized zero valent heterodiatomic compounds with main group elements and/or mixed transition metal-main group elements with detail characterization by various spectroscopic techniques and studies of their electronic properties and bonding situation. Homogeneous catalysis with cyclic alkyl(amino) carbene (cAAC)-transition metal complexes with low valent, low coordinate metal centers. Methodology development for the syntheses of biologically relevant small organic molecules using commercially available transition metal 1atalyst .

Educational and Professional Career

Ph.D (December, 2012): Institute of Organic Chemistry, University of Regensburg, Germany

Postdoctoral Fellow (February, 2013 - June, 2014): Institute of Organic and Biomolecular Chemistry, Georg-August-University Göttingen, Germany

Postdoctoral Fellow (July, 2014 - November, 2015): Institute of Inorganic Chemistry, Georg-August-University Göttingen, Germany

Assistant Professor (January, 2016 ~): Indian Institute of Science Education and Research (IISER) Tirupati, India

Honours and Awards

Deutscher Akademischer Austausch Dienst (DAAD) Fellowship (2009-2012) for Doctoral studies in Germany German Academic Exchange Service-DAAD

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

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Recent Picture

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Career Profile: Prof. Pinaki Talukdar completed his Ph.D. in Organic Chemistry from the University of Geneva, Switzerland in 2005. After completing a Postdoc from the University of Illinois at Urbana Champaign, USA (2005-2006), he worked as Senior Research Scientist at AMRI Global (Presently Curia Global), Hyderabad (2006-2007) and then at the Institute of Life Sciences (Presently Dr. Reddy's Institute of Life Sciences), Hyderabad (2007-2009). He joined the Chemistry Department of IISER Pune as Assistant Professor in 2009. He was promoted to Associate Professor in 2015, and Professor in 2020. He is also a Rahul Bajaj Chair Professor and Dean of Faculty at the Institute.

Awards/achievements: Prof. Talukdar is a recipient of DBT National Bioscience Award for Career Development in, 2016, CRSI Bronze Medal in 2018, and SERB Distinguished Investigator Award in 2019.

Selected Publications:

1. *A Glutathione Activatable Ion Channel Induces Apoptosis in Cancer Cells by Depleting Intracellular Glutathione Levels.* Javid Ahmad Malla, Virender Kumar Sharma, Mayurika Lahiri, Pinaki Talukdar. *Angew. Chem. Int. Ed.* **2020**, *26*, 11946-11949.
2. *Apoptosis-Inducing Activity of a Fluorescent Barrel-Rosette M^+/Cl^- Channel.* Javid Ahmad Malla, Rintu M. Umesh, Amal Vijay, Arnab Mukherjee, Mayurika Lahiri, Pinaki Talukdar.* *Chem. Sci.* **2020**, *11*, 2420-2428.
3. *Phototriggered Release of a Transmembrane Chloride Carrier from an o-Nitrobenzyl-Linked Procarrier.* Swati Bansi Salunke, Javid Ahmad Malla, Pinaki Talukdar* *Angew. Chem. Int. Ed.* **2019**, *58*, 5354-5358.
4. *A Dimeric Bis(melamine)-Substituted Bispidine for Efficient Transmembrane H^+/Cl^- Cotransport.* Sopan Valiba Shinde, Pinaki Talukdar.* *Angew. Chem. Int. Ed.* **2017**, *56*, 4238-4242.
5. *Chloride Transport through Supramolecular Barrel-Rosette Ion Channels: Lipophilic Control and Apoptosis-Inducing Activity.* Tanmoy Saha, Amitosh Gautam, Arnab Mukherjee, Mayurika Lahiri, Pinaki Talukdar.* *J. Am. Chem. Soc.* **2016**, *138*, 16443-16451.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Diverse Role of N-Heterocyclic Carbene Complexes of Cobalt: Application in Carbon-Boron Bond Formation

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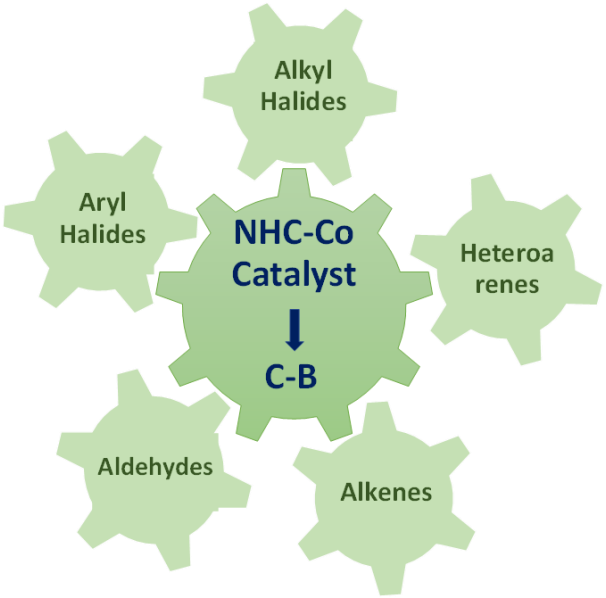
Abstract:
Given their importance in utility as versatile precursors to a wide range of other valuable families of molecules, introducing diverse functionality into the organoboron compounds will enhance its use as a synthetic handle in target-directed synthesis.[1] Several efficient synthetic routes has been established and most of them rely on heavy metal based catalysts such as Pd, Rh, Ir etc. which suffers from inherent toxicity, cost and sustainability concerns.[2] This obviously put forth the needful for the development of catalytic systems based on earth abundant metals like Mn, Fe, Co etc. We have developed *N*-heterocyclic carbene supported cobalt catalysts for the synthesis of variety of boronic ester derivatives using cheap as well as challenging precursors, such as aryl and alkyl halides[3,4], substituted alkenes,[5] N-heterocycles and aldehydes. The key results will be discussed.



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(1) *Boronic Acids: Preparation and Applications in Organic Synthesis, Medicine and Materials*; 2nd ed.; Hall, D. G., Ed.; Wiley-VCH: Weinheim, 2011.
(2) (a) Mkhalid, I. A. I.; Barnard, J. H.; Marder, T. B.; Murphy J. M.; Hartwig, J. F. *Chem. Rev.* **2010**, *110*, 890-931. (b) Neeve, E. C.; Geier, S. J.; Mkhalid, I. A. I.; Westcott, S. A.; Marder, T. B. *Chem. Rev.* **2016**, *116*, 9091-9161.
(3) Verma, P. K.; Mandal, S.; Geetharani, K. *ACS Catal.* **2018**, *8*, 4049-4054.
(4) Verma, P. K.; Sujit Prasad, K.; Varghese, D.; Geetharani, K. *Org. Lett.* **2020**, *22*, 1431-1436.
(5) Verma, P. K.; Sethulekshmi, A. S.; Geetharani, K. *Org. Lett.* **2018**, *20*, 7840-7845.

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Geetharani was born and raised in Madurai, Tamilnadu, India. She began her independent research career as an Assistant Professor at department of inorganic and physical chemistry, Indian Institute of Science Bangalore, India in 2016. She was promoted to an Associate professor in 2022. She is a recipient of DST-Inspire Faculty Award. She has been elected as Young Scientist/Affiliate by all three Science Academies in India. She received the SERB-Women Excellence Award from the President of India. She is also an Editorial member of Chemistry – An Asian Journal and a member of the Early Career Advisory Board of the European Journal of Inorganic Chemistry. Her research interests are in the areas of catalysis, main group and organometallic chemistry.

Representative Publications:

1. Verma, P. K.; Meher, N. K.; Geetharani, K.* Homolytic Cleavage of Diboron(4) Compounds by Diazabutadienes. *Chem Commun.* **2021**, *57*, 7886 – 7889. Highlighted on the Cover Page of the Article.
2. Siddiqui, S.; Bhawar, R.; Geetharani, K.* Iron-Based Catalyst for Efficient Borylation of Unactivated Alkyl Halides. *J. Org. Chem.* **2021**, *86*, 1948-1954.
3. Verma, P. K.; K. Sujit Prasad.; D. Varghese.; Geetharani, K.* Cobalt(I)-Catalyzed Borylation of Unactivated Alkyl Bromides and Chlorides. *Org. Lett.* **2020**, *22*, 1431-1436.
4. Verma, P. K.; Setulekshmi, A. S.; Geetharani, K.* Markovnikov-Selective Co(I)-Catalyzed Hydroboration of Vinylarenes and Carbonyl Compounds. *Org. Lett.* **2018**, *20*, 7840-7845.
5. Mandal, S.; Verma, P. K.; Geetharani, K.* Lewis Acid Catalysis: Regioselective Hydroboration of Alkynes and Alkenes Promoted by Scandium triflate. *Chem. Commun.* **2018**, *54*, 13690-13693. Highlighted in Synfacts **2019**, *15* (02), 0150.
6. Verma, P. K.; Souvik, M.; Geetharani, K.,* Efficient Synthesis of Aryl Boronates via Cobalt-Catalyzed Boryla-tion of Aryl Chlorides and Bromides. *ACS Catal.* **2018**, *8*, 4049-4054. Highlighted in Synfacts 2018, 14(07), 0746.

Estimation of Viscosity of Confined Water: Application of Translational Jump-diffusion Approach

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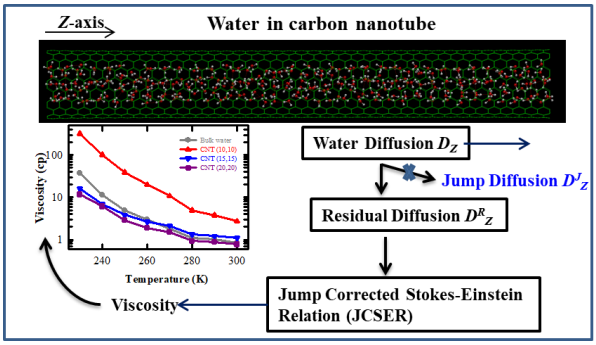
Abstract:
Estimation of viscosity of water under nanoscopic confinement is crucial for numerous applications in nanotechnology and biochemistry. The presence of confinement does not allow the viscosity to be estimated in the same way as is done with bulk water. The Stokes-Einstein relationship (SER), which links diffusion and viscosity, paved the way to predict viscosity quantitatively.[1] Unfortunately, under various conditions, such as low temperature, low pressure, SER severely breaks down.[2] We have proposed a new strategy based on our translational jump diffusion (TJD) approach[3-6], which has proven successful in quantitatively explaining SER breakdown in supercooled water and aqueous solution. In this approach, the translational jump-diffusion coefficient, which emanates from the translational jump (large amplitude displacement) of the molecules and contributes part of the total diffusion, is calculated using a quantitative manner. Interestingly, the remaining part of the diffusion remains coupled to the viscosity of the medium under all thermodynamic conditions. The above TJD-based approach uses the diffusion of the water molecules to predict the viscosity of water, confined in single walled carbon nanotube (CNT). It is observed that the confinement has much larger effect on water viscosity than previously predicted. In specifics, viscosity of water inside the 1.36 nm diameter CNT is nearly 3 times larger than that of the bulk water under the same thermodynamic conditions. The effect increases manifold in supercooled condition. For example. at 230 K, water in CNT is about 10 times more viscous than bulk water. Therefore, this work proposes a new approach to predict the viscosity of confined water under arbitrary conditions.



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3. Dueby, S.; Dubey, V.; Daschakraborty, S. Decoupling of Translational Diffusion from the Viscosity of Supercooled Water: Role of Translational Jump Diffusion. *J. Phys. Chem. B* **2019**, *123*, 7178– 7189
4. Dubey, V.; Erimban, S.; Indra, S.; Daschakraborty, S. Understanding the Origin of the Breakdown of the Stokes–Einstein Relation in Supercooled Water at Different Temperature–Pressure Conditions. *J. Phys. Chem. B* **2019**, *123*, 10089– 10099
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6. Dubey, V.; Dueby, S.; Daschakraborty, S. Breakdown of the Stokes–Einstein relation in supercooled water: the jump-diffusion perspective. *Phys. Chem. Chem. Phys.* **2021**, *23*, 19964– 19986

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Career Profile, significant awards/achievements and representative publications

Dr. Snehasis Daschakraborty is an Assistant Professor in the Dept. of Chemistry, Indian Institute of Technology (IIT) Patna, India. He completed his Ph.D. in 2014 from S. N. Bose National Center for Basic Sciences, Kolkata, India. After 3 years of postdoctoral research in the University of Colorado, Boulder, USA, he started his independent career at IIT Patna from December, 2016. His group works in the area of structure and dynamics of liquid and bimolecular systems.

He has published more than 40 papers in various journals of good repute in his entire research career so far. His works have been recognized by various science academies in India. He was the recipient of INSA medal for young scientist 2020. He is an elected Member of National Academy of Science, India (M. N. A. Sc.). Phys. Chem. Chem. Phys. (RSC Journal) also recognized him as an *emerging investigator* and invited to contribute in the special issue, namely "2021 PCCP Emerging Investigators themed collection". Following are some of his representative publications in his independent career.

1. Maiti et al. *J. Phys. Chem. B* **2022,** *126* (7), 1426-1440.
2. Dubey et al., *J. Phys. Chem. B* **2022,** *126* (12), 2430-2440.
3. Maiti et al. *J. Phys. Chem. B* **2021,** *125* (36), 10149-10165.
4. Maiti et al., *J. Phys. Chem. B* **2021,** *125* (4), 1167-1180.
5. Dubey et al., *Phys. Chem. Chem. Phys.* **2021,** *23* (36), 19964-19986.
6. Erimban et al., *Phys. Chem. Chem. Phys.* **2021,** *23* (48), 27294-27303.
7. Erimban et al., *Advanced Materials Interfaces* **2021,** *8* (13), 2170073.
8. Erimban et al., *J. Phys. Chem. Lett.* **2020,** *11* (18), 7709-7716.
9. Dubey et al., *J. Phys. Chem. B* **2020,** *124* (46), 10398-10408.
10. Erimban et al., *Phys. Chem. Chem. Phys.* **2020,** *22* (11), 6335-6350.
11. Dueby et al., *J. Phys. Chem. B* **2019,** *123* (33), 7178-7189.
12. Dubey et al., *J. Phys. Chem. B* **2019,** *123* (47), 10089-10099.
13. Verma, et al. *J. Phys. Chem. C* **2019**, *123*, 16681-16689.
14. Erimban et al., *J. Chem. Phys.* **2019,** *151*, 065104.
15. Dubey et al., *Phys. Chem. Chem. Phys.* **2019,** *21* (2), 800-812.
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17. Daschakraborty, S., *J. Chem. Phys.* **2018,** *148* (13), 134501.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Prof. Raakhi Gupta

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Raakhi Gupta obtained her Ph.D. on the topic "Some new organophosphorus compounds containing dicoordinated phosphorus atom" in 1995 from University of Rajasthan, Jaipur (India). Presently she is a Professor of Chemistry at IIS (Deemed to be University), Jaipur (India).

A highly meritorious student, a gold medallist, Dr. Gupta has had an illustrious academic career, which includes a Summer Research Fellowship of the Indian Academy of Sciences at IIT, Mumbai and a Summer School at New Hampshire, USA, among many others. She is actively involved in research and has about 33 research papers published in National and International Journals of repute, besides guiding 8 Ph.D. scholars she has also presented papers abroad in international conferences and in India as well. Her current research interests include organophosphorus chemistry, synthetic organic chemistry and computational chemistry with an emphasis on determination of reaction mechanism. Currently she is also the coordinator of two Erasmus + funded projects, Tuning India and Tuning RISHII in which IIS University partnering with University of Deusto, Bilbao, Spain.

She has been bestowed upon several awards including Women's Progression Award (in recognition of her contribution in the field of education), Avantika Shikshak Samman (Avantika Teachers' Felicitation) etc. Recently, she received Change Maker Humanity Award in Edu-Leader category (University), presented by Bharat Soka Gakkai in recognition of her outstanding efforts and contribution in the field of education

FEW RECENT PUBLICATIONS

1. **Review:** "Recent advances in organocatalytic asymmetric aza-Michael reactions of amines and amides", Pratibha Sharma, **Raakhi Gupta** and Raj K. Bansal, ***Beilstein J. Org. Chem***. 2021 *17*, 2585–2610. https://doi.org/10.3762/bjoc.17.173
2. "A new cross-conjugated mesomeric betaine", Nivedita Sharma, Manjinder Kour, **Raakhi Gupta** and Raj K. Bansal, ***RSC Adv.***, **2021**, *11*, 25296. DOI: 10.1039/d1ra03981d
3. "N-Heterocyclic Carbenes–Cu(I) Complexes as Catalysts: A Theoretical Insight", Nosheen Beig, Varsha Goyal, **Raakhi Gupta**, and Raj K. Bansal, ***Aust. J. Chem.***, **2021, *74***, 503. DOI: 10.1071/CH20332
4. "Michael addition of ethyl anthranilate and phenyl monothioanthranilate to acetylenic esters: experimental and theoretical results", Pratibha Sharma, **Raakhi Gupta**, R. K. Bansal, ***Struct Chem*, 2021,** *32*, 1611. doi.org/10.1007/s11224-021-01735-9
5. "A DFT Investigation of the retro-ene reactions of β-hydroxyacetylenes: Concerted or stepwise mechanism" **Raakhi Gupta**, R. K. Bansal, ***Struct Chem*, 2020,** *31*, **351.** doi.org/10.1007/s11224-019-01410-0

Biophysical Insight Into FnCas9 Editor Linked Uniform Detection Assay (FELUDA): FELUDA-V2

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& CSIR-National Chemical Laboratory, Pune
Adjunct Professor, *Indian Institute of Science Education and Research Mohali*
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The present invention describes a method for using a bacterial CRISPR Cas Ribonucleoprotein complex for detecting any DNA or RNA fragment, without the need for sequencing. The principle of detection is derived from the natural property of the enzyme being used for the invention, Francisella novicida Cas9 (fnCas9) which shows very low binding affinity to mismatched substrates. DNA is isolated either from blood, saliva, or any other biological sources like bacteria and amplified if required. For virus infected patients, samples are collected as a nasal swab and inactivated. Total RNA isolated from the sample is converted to cDNA using the reverse transcriptase enzyme. The DNA (when test material is DNA) or cDNA (when test material is RNA, like for COVID-19) is subjected to Polymerase Chain reaction, amplifying using specific primers and tagging the amplified DNA products with a ligand of choice. The detection mix consists of labelled PCR products, sgRNA-fnCas9 complex. The detection complex can be visualized using a wide array of technologies like lateral flow, gel based cleavage assay, fluorescence based detection, in both low, medium or plate based high-throughput format. Science behind this technology will be discussed in the presentation.

1. FnCas9 based CRISPR diagnostic for rapid and accurate detection of major SARS-CoV2 variants on a paper strip. Kumar M, Gulati S, Ansari AH, Phutela R, Acharya S, Azhar M, Murthy J, Kathpalia P, Kanakan A, Maurya R, Vasudevan JS, Murali A, Pandey R, Maiti S, Chakraborty D. ***Elife***. 2021 Jun 9;10:e67130. doi: 10.7554/eLife.67130.

2. Rapid and accurate nucleobase detection using FnCas9 and its application in COVID-19 diagnosis. Azhar M, Phutela R, Kumar M, Ansari AH, Rauthan R, Gulati S, Sharma N, Sinha D, Sharma S, Singh S, Acharya S, Sarkar S, Paul D, Kathpalia P, Aich M, Sehgal P, Ranjan G, Bhoyar RC; Indian CoV2 Genomics & Genetic Epidemiology (IndiCovGEN) Consortium, Singhal K, Lad H, Patra PK, Makharia G, Chandak GR, Pesala B, Chakraborty D, Maiti S. ***Biosens Bioelectron***. 2021 Jul 1;183:113207. doi: 10.1016/j.bios.2021.113207.

3. Low-cost CRISPR diagnostics for resource-limited settings. Gulati S, Maiti S, Chakraborty D. ***Trends Genet***. 2021 May 17:S0168-9525(21)00129-3. doi: 10.1016/j.tig.2021.05.001.
4. Rapid identification and tracking of SARS-CoV-2 variants of concern. Chakraborty D, Agrawal A, Maiti S. ***Lancet*** 2021 Apr 10;397(10282):1346-1347. doi: 10.1016/S0140-6736(21)00470.

5. Francisella novicida Cas9 interrogates genomic DNA with very high specificity and can be used for mammalian genome editing. Acharya S, Mishra A, Paul D, Ansari AH, Azhar M, Kumar M, Rauthan R, Sharma N, Aich M, Sinha D, Sharma S, Jain S, Ray A, Jain S, Ramalingam S, Maiti S, Chakraborty D. ***Proc Natl Acad Sci U S A***. 2019 Oct 15;116(42):20959-20968.
6. CRISPR/Cas9: a historical and chemical biology perspective of targeted genome engineering. Singh A, Chakraborty D, Maiti S. ***Chem Soc Rev***. 2016 Dec 21;45(24):6666-6684.

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Souvik Maiti completed his B. Sc. (1993) And M. Sc (1995) in Chemistry from Jadavpur University, Kolkata, and PhD (1999) in synthetic polymer chemistry from the CSR-Indian Institute of Chemical Technology, Hyderabad, India. After post-doctoral training from College of Pharmacy, UNMC, Omaha, USA and Department of Physics, Curie Institute, Paris, France, he joined as a research faculty CSIR-Institute of Genomics and Integrative Biology, Delhi, in 2003. He is also adjunct research faculty in CSIR-National Chemical Laboratory, Pune and adjunct professor in the Indian Institute of Science Education and Research (IISER) Mohali.

He works in the interface of Chemistry and Biology and focuses on the chemical biology of nucleic acids to address questions of importance in biology and medicine. Currently his research group is engaged in developing potent Indigenous CRISPR-Cas9 based tools for point-of care diagnostics and for the cheaper treatment of genetic diseases. Recently he is part of a team that has initiated a 5-year clinical trial to evaluate the indigenously developed CRISPR/Cas9 gene editing tool as a potential cure for sickle cell disease.

Catalytic Oxidation of Biothiols in Cancer Cells: A New Strategy for Designing Catalytic Anticancer Agents

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Cancer remained one of the leading causes of mortality with 10 million deaths in 2020.[1] The most widely used clinical treatment modality is cytotoxic chemotherapy using platinum drugs which is used to treat variety of cancers. However, inherent or acquired chemo-resistance in cancer cells and dose-limiting toxic side effects (e.g. nephrotoxicity, neurotoxicity, etc.) arising from indiscriminate killing of cancerous and non-cancerous cells severely limit the efficacy of currently used chemotherapy.[2] To tackle these drawbacks, a novel Re (VII)-oxo catalytic anticancer agent was developed in our lab (Figure 1).[3] Being stable in biological media, the catalyst efficiently enters inside cells and oxidises intracellular thiols such as GSH utilizing endogenously produced H_2O_2 as primary oxidant. The catalyst possesses potent and selective anticancer activity arising from its ability to induce oxidative stress through misbalancing cellular redox homeostasis. The catalyst is able to circumvent platinum resistant in ovarian, lung, and prostate cancer cells. Mechanistic studies revealed that the catalyst accumulates preferentially in cytoplasm, upregulates intracellular ROS, depletes mitochondrial membrane potential and induces ER-stress, that trigger apoptosis in cancer cells. I will discuss the design, synthesis, catalysis and biological evaluation of the novel Re (VII)-oxo catalytic anticancer agent.

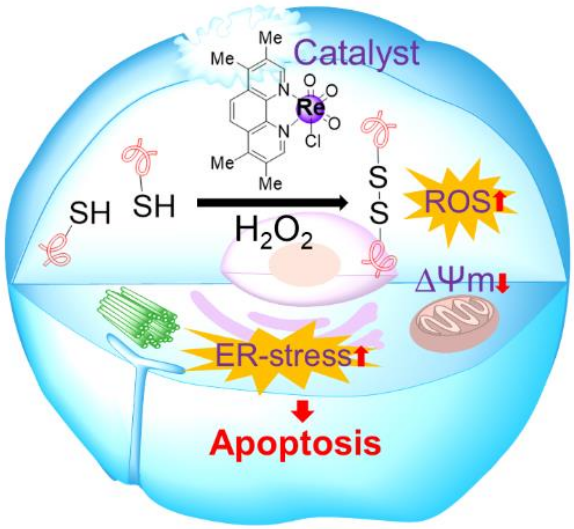

Figure 1. Mechanism of anticancer activity of the Re(VII)-oxo catalytic anticancer agent.

References and Notes:

1. Vaidya, S. P.; Gadre, S.; Kamisetti, R. T.; Patra, M. *Biosci. Rep.* **2022**, *42*, BSR20212160.
2. Johnstone, T. C.; Suntharalingam, K.; Lippard, S. *J. Chem. Rev.* **2016**, *116*, 3436-3486.
3. Das, S.; Patra, M. *Submitted*., **2022**.

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Career Profile

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Department of Chemical Sciences, Tata Institute of Fundamental Research, India

08/2018-continuing

Previous appointments:

Senior Scientist: University of Zurich, Switzerland 12/2015-08/2018

Post-Doctoral Fellow: Massachusetts Institute of Technology, 09/2013-11/2015

Post-Doctoral Fellow: University of Zurich, Switzerland 09/2011-08/2013

Education:

PhD: Ruhr University Bochum, Germany, 2011

MSc: Indian Institute of Technology, Bombay, 2007

Representative publications:

- A Rationally Designed Bimetallic Platinum (II)-Ferrocene Antitumor Agent Induces Non-Apoptotic Cell Death and Exerts in Vivo Efficacy.

  S. Gadre, M. Manikandan, P. Duari,S. Chhatar, A. Sharma, M. Kumar, U. Kolthur-Seetharam, Malay Patra*, Chem. Eur. J., 2022, DOI: 10.1002/chem.202201259.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

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Academic and Professional Background:

2020- Professor, IISER Pune
05-07/2019 AvH Fellow, TUM, Germany. (Host: Prof. Roland A. Fischer)
2009-2015 and 2015-2020: Assistant and Associate Professor, IISER Pune
2007-2009 JSPS and CREST PDF, Kyoto University, Japan. (Host: Prof. Susumu Kitagawa)
2006 - PhD in Chemistry, IIT, Kanpur (Supervisor: Prof. Parimal K. Bharadwaj)
2001 - M.Sc. (Inorganic Chemistry), Banaras Hindu University (BHU), Varanasi, India
1999 - B.Sc., Burdwan University (Ramananda College, Bishnupur, Bankura, W. B., India)

Awards/Recognition/Fellowships:

2020-Advisory Board of ChemCommun,
2020-Materials Research Society of India (MRSI) Medal,
2019-India Research Excellence - Citation (Young Researcher) Award by Clarivate Analytics,
2018-Alexander von Humboldt (AvH) Fellowship for Experienced Researchers, Germany.

Representative publications:

Energy & Environmental Science 2022, (Just accepted)
Angew. Chem. Int. Ed. 2022, DOI: 10.1002/anie.202203385.
Angew. Chem. Int. Ed. 2022, 61, e202114132.
ACS Cent. Sci. 2020, 6, 9, 1534–1541.
Angew. Chem. Int. Ed. 2020, 59, 7788.
Coord. Chem. Rev. 2019, *395*, 146-192.
Accounts of Chemical Research 2017, 50, 2457-2469.
Chem. Soc. Rev. 2017, *46*, 3242-3285.

Connecting the dots: preporous molecules to porous organic polymers

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Abstract: Porous organic molecules (POMs), such as organic cages and cavitands, are well-known for guest-recognition properties and enzyme-mimetic catalysis.[1] On the other hand, porous organic polymers (POPs) have attracted significant attention in the last few years for their potential applications in heterogeneous catalysis and water purification due to their high porosity, customizable structures, and outstanding hydrothermal stability.[2] Knitting the preporous POMs with zero-dimensional pores using rigid aromatic linkers leads to a new generation of three-dimensional porous polymers where intrinsic properties of the POMs can be amalgamated with highly porous and robust POPs.[3] Thus, the 'cavitand/cage-to-network' approach can open up an interesting field of research where we can address many unresolved problems related to sustainable development and environmental remediation. In this talk, I shall discuss the catalytic performance of various organic cavitands and cage-based POPs developed in our group (e.g., resorcin[4]arene cavitand, waterwheel-like noria cage) for chemical fixation of CO_2 and size-selective, charge-specific separation of organic micropollutants from water.[3]

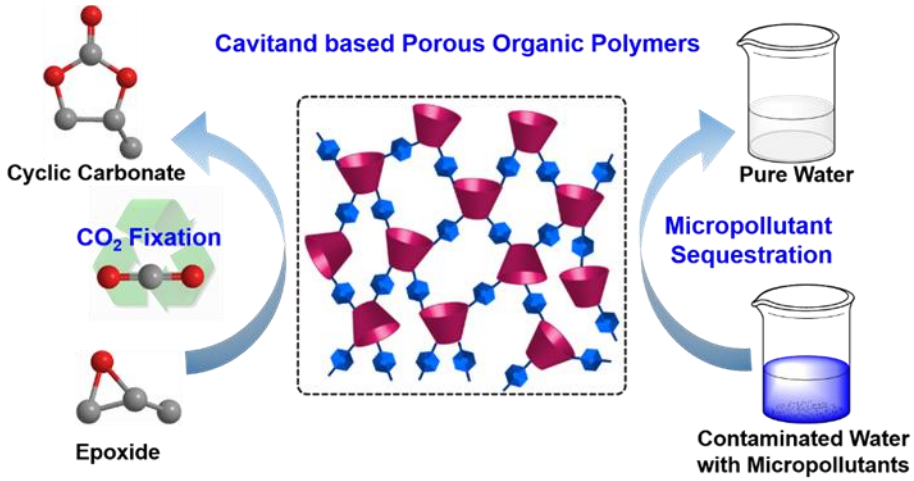

Figure: Connecting zero-dimensional cavitands/cages with rigid aromatic linkers leading to 3D-porous organic polymers (POPs) for catalytic fixation of CO_2 and micropollutant removal from water.

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Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch

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- **Current Position(s)**

April 2018 – Present: Associate Professor, Department of Chemistry, IISER Bhopal
July 2012 – March 2018: Assistant Professor, Department of Chemistry, IISER Bhopal

- **Previous Positions**

Sept, 2010 – June 2012: Alexander von Humboldt fellow
Dept. of Macromolecular Chemistry, University of Wuppertal, Germany
June 2009 – June 2010: Post-doctoral fellow in PPSM, ENS Paris-Saclay, France

- **Fellowships And Awards**

2023: Chemical Research Society of India (CRSI) Bronze Medal
2018: Emerging Investigator: *Journal of Material Chemistry C* (Royal Society of Chemistry)
Sept, 2010 – June 2012: Alexander von Humboldt Fellowship awarded in Materials Science

- **Representative publications**

1. A. Giri, S. Biswas, M. W. Hussain, T. K. Dutta, A. Patra,* Nanostructured Hypercrosslinked Porous Organic Polymers: Morphological Evolution and Rapid Separation of Polar Organic Micropollutants, *ACS Appl. Mater. Interfaces* **2022**, *14*, 7369-7381.
2. B. Sk, M. Sarkar, K. Singh, A. Sengupta, A. Patra,* UV to NIR Multistate Electrochromism and Electrofluorochromism in Dibenzophenazine-arylamine Derivatives, *Chem. Commun.* **2021**, *57*, 13590-13593.
3. S. Kundu, A. Chowdhury, S. Nandi, K. Bhattacharyya,* A. Patra,* Deciphering the Evolution of Supramolecular Nanofibers in Solution and Solid-state: A Combined Microscopic and Spectroscopic Approach, *Chem. Sci.* **2021**, *12*, 5874-5882.
4. A. Giri, N. N. Patil, A. Patra,* Porous Noria Polymer: A Cage-to-Network Approach toward a Robust Catalyst for CO_2 Fixation and Nitroarene Reduction, *Chem. Commun.* **2021**, *57*, 4404-4407.
5. B. Sk, S. Sharma, A. James, S. Kundu, A. Patra,* N-rich Electron Acceptors: Triplet Harvesting in Multichromophoric Pyridoquinoxaline and Pyridopyrazine-based Organic Emitters, *J. Mater. Chem. C* **2020**, *8*, 12943-12950.
6. M. W. Hussain, V. Bhardwaj, A. Giri, A. Chande,* A. Patra,* Multifunctional Ionic Porous Frameworks for CO_2 Conversion and Combating Microbes, *Chem. Sci.* **2020**, *11*, 7910-7920.
7. S. Kundu, B. Sk, P. Pallavi, A. Giri, A. Patra,* Molecular Engineering Approaches towards All-organic White Light Emitting Materials, *Chem. Eur. J.* **2020**, *26*, 5557-5582.
8. A. Giri, M. W. Hussain, B. Sk, A. Patra,* 'Connecting the Dots': Knitting *C*-phenylresorcin[4]arenes with Aromatic Linkers for Task-specific Porous Organic Polymers, *Chem. Mater.* **2019**, *31*, 8440-8450.

Elucidation of Naphthol-Derived 'ONO' Ligands and Their Transition Metal Complexes as a source of Oxidative Stress Induction and Insight into the Mechanism of Action

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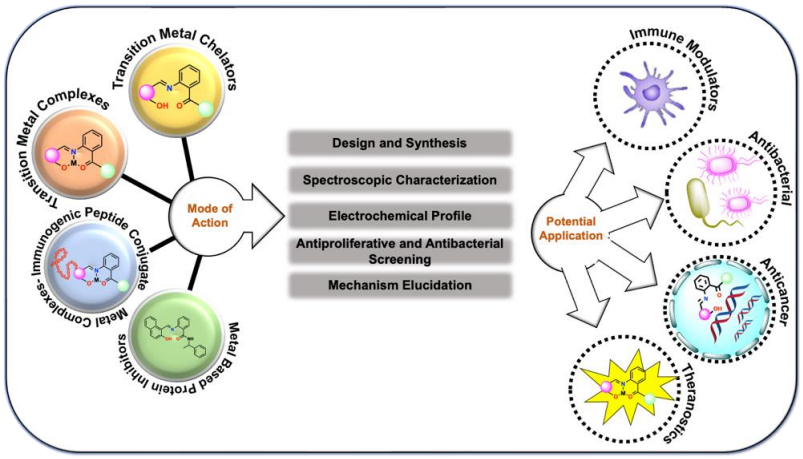
Abstract:
Trace metals are essential micronutrients required for survival across all three domains of life. From bacteria to animals, metals serve as structural and catalytic cofactors for approximately one-third of the proteome, constituting a major factor in the maintenance of cellular homeostasis. Metal ions' and their complex's reactivity confers upon them the ability to stimulate enzyme catalysis and stabilize reaction intermediates. However, these properties render metals toxic at high concentrations, necessitating strict regulation of metal levels. Having evolved in close association with several classes of biologically relevant metal chelators, we have developed numerous strategies for the utilization of these metal chelators to limit metal availability and thereby prevent bacterial, cancer, and viral proliferation.
Herein, we targeted Histone Deacetylases (HDAC) and Ribonucleotide Reductase (RNR) Enzyme inhibitors and synthesized a library of more than 400 novel 'ONO' and 'NO' binding site ligands with substituted benzyl/naphthyl moiety and their corresponding transition metal complexes with Fe(II), Fe(III), Ni(II), Cu(II), and Zn(II). We explored the cell-specific and strain-specific roles of these distinct ligands and their metal complexes in shaping cancer and bacterial infections, as well as implications for new therapeutic development. Few compounds revealed a high MIC value against *S.aureus* in the low nanomolar concentration range. The high anticancer/antibacterial activity of the lead drug candidate is linked to metal deprivation and reactive oxygen species induction, which was further confirmed by several in-vitro and spectroscopic experiments.



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Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

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Bio-Sketch of Speaker

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1. B.Sc. Banaras Hindu University, Varanasi, 2006 - 09.
2. M.Sc., Indian Institute of Technology Delhi, 2010 - 12.
3. PhD., The University of Arizona, USA, 2012-17.
4. Research Associate: The Scripps Research Institute, California, USA, 2017-19.
5. Designated Campus Colleague: The University of Arizona, Tucson, USA, 2017-19.
6. Assistant Professor: IIT Kanpur, Sep 2019 - ongoing

Awards and Honours:

1. INSPIRE Faculty Fellowship
2. The ACS Southern Arizona Section Women Chemist Group 1st Place ACS Award
3. Carl S. Marvel Memorial Fellowship
4. David F. O'Brien Scholar in Chemistry
5. Galileo Circle Scholar

Publications:

1. Gautam, R.; Loughrey, J. J.; Astashkin, A. V.; Shearer, J.; Tomat, E. "Tripyrrindione as a redox-active ligand: Palladium (II) coordination in three redox states". Angewandte Chemie, 2015, 127, 15107-15110
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3. Gautam, R.; Astashkin, A. V.; Chang, T. M.; Shearer, J.; Tomat, E. "Interactions of Metal-Based and Ligand-Based Electronic Spins in Neutral Tripyrrindione π-Dimers" Inorganic Chemistry, 2017, 56, 6755–6762.
4. Gautam, R.; Petritis, S. J.; Astashkin, A. V.; Shearer, J.; Tomat, E. "Zinc binding by redox-active biopyrrin ligands: Paramagnetism and fluorescence of zinc(II) tripyrrindione" 2018, Inorganic Chemistry, 2018.

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Career Profile:

Devarajulu Sureshkumar did his B. Sc. in Chemistry and M. Sc. in Organic Chemistry at the University of Madras. He obtained his Ph.D. under the supervision of Prof. S. Chandrasekaran, Department of Organic Chemistry, IISc Bangalore, in 2007. He worked with Dr. Martin Klussman in Prof. Benjamin List's group at the Max-Planck-Institut für Kohlenforschung, Germany as an AvH postdoctoral fellow from 2008 to 2010. After a short stay as a postdoctoral associate with Prof. Wilhelm Boland at the Max-Planck-Institut for Chemical Ecology in Jena, Germany, he moved to Japan as a JSPS fellow to work with Prof. Masakatsu Shibasaki at the Institute of Microbial Chemistry in Tokyo (2010-2015). He joined the IISER Kolkata as a faculty in the Department of Chemical Sciences in February 2015. Currently, his lab is focusing on visible-light-mediated photocatalysis for C–C bond-forming and fluorination reactions using C(sp^3)–H functionalization.

Significant awards/achievements:

Early Carrier Research Award (2017) from SERB, Government of India.
Ramanujan Fellowship (2016) from SERB/DST, Government of India.
JSPS Fellowship (2013) for Foreign Researchers (Pathway to University Positions in Japan).
JSPS Fellowship (2011) at Institute of Microbial Chemistry, Tokyo, Japan.
AvH Fellowship (2008) at Max-Planck Institute for Khölenforschung, Germany.

Representative publications:

1. Diastereoselective Palladium-Catalyzed C(sp^3)–H Cyanomethylation of Amino Acid and Carboxylic Acid Derivatives. Garai, S.; Ghosh, K. G.; Biswas, A.; Chowdhury, S.; Sureshkumar, D. *Chem. Commun*. **2022**, xx, xxx. DOI: org/10.1039/D2CC03106J.
2. Visible-Light Photoredox Catalyzed Decarboxylative Alkylation of Vinylcyclopropanes. Chandu, P.; Das, D.; Ghosh, K. G.; Sureshkumar, D. *Adv. Synth. Catal*. **2022**, 364, 1-7. VIP Article.
3. Visible-Light Driven Organo-photocatalyzed Multicomponent Approach for Tandem C(sp^3)–H Activation and Alkylation Followed by Trifluoromethylthiolation. Ghosh, K. G.; Das, D.; Garai, S.; Chandu, P.; Sureshkumar, D. *J. Org. Chem*. **2022**, *87*, 8611-8622.
4. TEMPO-Mediated Regioselective Synthesis of Isoxazolines, 5-Hydroxy-2-isoxazolines, and Isoxazoles via Aliphatic δ-C(sp^3)–H Bond Oxidation of Oximes. Mondal, S.; Biswas, S.; Ghosh, K. G.; Sureshkumar, D. *Chem. Asian. J.* **2021**, *16*, 2439-2446. Special Issue on "15th Anniversary of IISER Inception".
5. Visible-Light-Driven Organophotocatalyzed Mono-, Di-, and Tri-C(sp^3)–H Alkylation of Phosphoramides. Ghosh, K. G.; Das, D.; Chandu, P.; Sureshkumar, D. *J. Org. Chem*. **2021**, 86, 2644-2657.
6. Ammonium Chloride-Mediated Trifluoromethylthiolation of p-Quinone Methides. Das, D.; Ghosh, K. G.; Chandu, P.; Sureshkumar, D. *J. Org. Chem*. **2020**, *85*, 14201-14209.
7. Metal-free Visible Light Promoted Trifluoromethylation of Vinylcyclopropanes Using Pyrylium Salt as Photoredox Catalyst. Chandu, P.; Ghosh, K. G.; Sureshkumar, D. *J. Org. Chem.* **2019**, *84*, 8771-8781.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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New Advances in Atomically Precise Silver Nanoclusters

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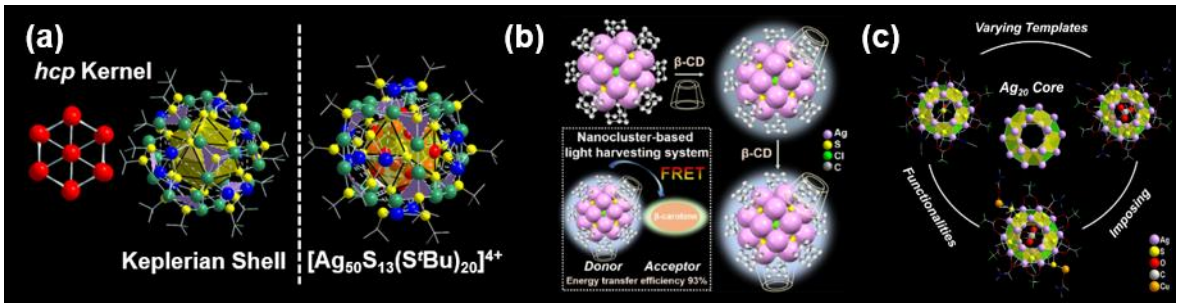
Abstract:
Atomically precise metal nanoclusters, a new class of materials are composed of tens to hundreds of metal atoms in the core possess unique structures, high stability and attractive properties. Built on the significant success of Au nanoclusters, Ag nanoclusters have recently received increasing attention. Synthesis and structural elucidation of Ag NCs is challenging because the zero-valent oxidation state of Ag is very reactive and prone to oxidization.[1] We have designed new strategy to synthesize novel silver clusters. Then we have adopted different methods to generate functionality and correlate their structure-property relationship. Here we will discuss three new silver nanoclusters and these are: (a) A new Ag-S cluster $[Ag_{50}S_{13}(S^tBu)_{20}][CF_3COO]_4$ with its unique hcp Ag_{14} kernel and Ag_{36} Keplerian shell-based structural architecture and its photoresponsivity;[2] (b) Anion template-assisted Ag_{16} silver nanocluster for artificial light-harvesting system through supramolecular functionalization;[3] (c) new approach for generating functionality in template-assisted alloying of atom-precise silver nanocluster.[4]



Scheme 1. (a) Structural anatomy of Ag_{50}; (b) artificial light-harvesting system using Ag_{16} cluster; (c) template-assisted alloying of Ag_{20} nanoclusters.

References and Notes:

1. Yang, J.; Jin, R. *ACS Mater. Lett.* **2019**, *1*, 482-489.
2. Biswas, S.; Das, A. K.; Reber, A. C.; Biswas, S.; Bhandary, S.; Kamble, V. B.; Khanna. S. N.; Mandal, S; *Nano Lett.* **2022**, *22*, 3721-3727.
3. Das, A. K.; Biswas, S.; Manna, S. S.; Pathak, B.; Mandal, S; *Chem. Sci.* **2022**, DOI: 10.1039/D2SC02786K.
4. Das, A. K.; Biswas, S.; Manna, S. S.; Pathak, B.; Mandal, S; Manuscript submitted.

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Sukhendu received his Doctoral degree from Solid State and Structural Chemistry Unit, Indian Institute of Science Bangalore, India in 2007, and was a post-doctoral research scholar at The Pennsylvania State University, USA during 2008-2012. He joined Indian Institute of Science Education and Research Thiruvananthapuram (IISER TVM), Kerala, India in 2012 as an Assistant Professor in the department of Chemistry and then promoted to Associate professor in 2017. His primary research interest is on atom-precise metal nanoclusters and metal-organic framework to explore their photo-physical and chemical properties with the emphasis on energy and environment. He has published more 100 papers in the international peer review journals and contributed to 5 book chapters. He is the recipient of CRSI Bronze medal on 2021 and recently inducted as Fellow of Royal Society of Chemistry through the leader in the Field.

Selected Publications:

1. A. K. Das, S. Biswas, S. S. Manna, B. Pathak, S. Mandal*, "Atomically Precise Silver Nanocluster for Artificial Light-Harvesting System Through Supramolecular Functionalization", ***Chem. Sci.*** **2022**, https://doi.org/10.1039/D2SC02786K
2. A. K. Das, S. Biswas, V. S. Wani, A. S. Nair, B. Pathak, S. Mandal*, "$[Cu_{18}H_3(S\text{-}Adm)_{12}(PPh_3)_4Cl_2]$: fusion of Platonic and Johnson solids through a Cu(0) center and its photophysical properties", ***Chem. Sci.*** **2022**, *13*, 7616-7625
3. S. Biswas, A. K. Das, A. C. Reber, S. Biswas, S. Bhandary, V. B. Kamble, S. N. Khanna, S. Mandal*. "The New Ag–S Cluster $[Ag_{50}S_{13}(S^tBu)_{20}][CF_3COO]_4$ with a Unique hcp Ag_{14} Kernel and Ag_{36} Keplerian-Shell-Based Structural Architecture and Its Photoresponsivity" ***Nano Lett.*** **2022**, *22*, 3721–3727
4. S. Gratious, A. S. Nair, S. Mukherjee, N. Kachappilly, B. Pathak, S. Mandal*, "Gold Deassembly: From $Au_{44}(SPh\text{-}^tBu)_{28}$ to $Au_{36}(SPh\text{-}^tBu)_{24}$ Nanocluster through Dynamic Surface Structure Reconstruction" **J. *Phys. Chem. Lett*. 2021**, *12*, 10987–10993.
5. A. K. Das, S. Mukherjee, S. S. Sreehari, A. S. Nair, S. Bhandary, D. Chopra, D. Sanyal, B. Pathak, and S. Mandal*, "Defects Engineering on Ceria and C-C Coupling Reactions Using $[Au_{11}(PPh_3)_7I_3]$ Nanocluster: A Combined Experimental and Theoretical Study", ***ACS Nano***, **2020** 14, 16681-16688.
6. M. P. Maman, A. S Nair, A. M Abdul Hakkim Nazeeja, B. Pathak, S. Mandal*, "Synergistic Effect of Bridging Thiolate and Hub Atoms for the Aromaticity Driven Symmetry Breaking in Atomically Precise Gold Nanocluster". ***J. Phys. Chem. Lett.***, ***2020***, *11*, *10052-10059.*

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

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Stereoselective Synthesis of Vinyl Heteroarenes & Conjugated Dienes via Zweifel Olefination

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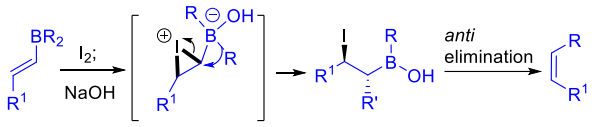
Abstract:

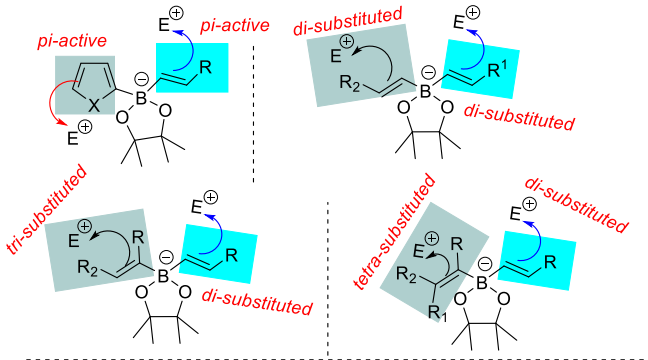
Zweifel olefination is an attractive transition metal-free method for the stereoselective synthesis of olefin. In the original method, the *E*-vinylboranes (derived from alkyne via hydroboration) can be converted into *Z*-alkenes by the addition of iodide and sodium hydroxide in THF medium (Scheme 1a). Although several developments have been made in the Zweifel olefination and its extension to heterocyclic synthesis, the chemistry remains mostly reserved either between a *pi*-inactive and *pi*-active system (alkyl/phenyl lithium with vinyl boronic ester or al-kyl/phenyl boron compound with vinyl lithium) or using similar olefin on both sides to control the stereoselectivity. The reactivity between two unsymmetrical olefins or between a heteroaryl and vinyl boronates is mostly unknown, which undermines its scope and impacts in organic synthesis. We have developed a stereoselective 1,2-migration from a substituted vinyl and hetroaryl boronate complex, which has produced *cis*-or *trans*-vinyl hetaroaryls, an important skeleton present in bioactive compounds and natural products. The reaction tolerated to furan, thiophene, indole, benzothiophene, and pyrroles. We have conducted theoretical calculation to understand the stereoselectivity.

a. Zweifel olefination for the synthes of Z-olefin via *anti*-elimination



b. Our work; Zweifel olefination using boron ate carrying two different active *pi*-system steric vs electronic effect

What controls the stereoselective 1,2-migration?



Scheme 1. Zweifel Olefination

References

a. Zweifel, G.; Arzoumanian, H.; Whitney, C. C. *J. Am. Chem. Soc.* **1967**, 89, 3652; b. Bonet, A.; Odachowski, M.; Leonori, D.; Essafi, S. Aggarwal, V. K. *Nat. Chem.* **2014**, *6*, 584; c) Paul, S.; Das, K. K.; Manna, S.; Panda, S. *Chem. Eur. J.* **2020**, 26, 1922.

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Dr. Santanu Panda obtained his PhD on 2013 in organocatalysis and total synthesis of natural products under Prof. Antony Pearson, Case Western Reserve University, Cleveland, USA. After finishing his PhD, he moved to Dallas and joined Prof. Joseph Ready group as postdoc. During his postdoc, he was exposed to transition metal catalysed cross coupling and organoboron chemistry. On July 2018, he joined IIT Kharagpur as an assistant professor. His group is very much active in organoboron chemistry, total synthesis of natural product and organophotoredox chemistry.

Awards / Honors / Membership:

- Ramanujan Fellowship 2018 from SERB
- Best Poster Award at UTSW Biochemistry Retreat at Dallas Botanical Garden, Dallas On 2017.
- Invited seminar to the annual UTSW Biochemistry department seminar series at UT Southwestern Medical Center, Dallas.
- Graduate outstanding teaching assistant award 2013, Department of Chemistry, Case Western Reserve University, USA.

Representative Publications:

Chem. Eur. J. **2020**, *26*, 1922;
Chem. Eur. J. **2020**, *26*, 14270
Org. Biomol. Chem., **2020**, *18*, 8939
Chem. Commun., **2021**, *57*, 441
Adv. Synth. Catal. **2021**, *363*, 2444
Coord. Chem. Rev. **2021**, 448, 214165
Org. Chem. Front., **2022**, *9*, 838
Chem. Rec. **2022**, 22, *e202100290*
Chem. Eur. J. **2022**, accepted
Eur. J. Org. Chem. **2022**, accepted

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
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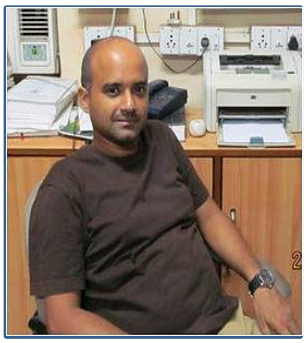
Samik Nanda

Professor



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Dr. Nanda completed his Ph.D. in 2002 at IICT-Hyderabad (with Dr J. S. Yadav) working on the theme ‘‘applications of enzymes in asymmetric organic synthesis’’. After completing two successive post-doctoral assignments (i) Texas A & M University, USA, with Prof. A. Ian Scott in the area of “*Genetically engineered synthesis of taxoids*” (ii) Toyama Prefectural University, Japan, (JSPS fellow with Prof. Y. Asano working in the area of “*Asymmetric catalysis with HNLs*”), he started his independent academic career at IIT Kharagpur in 2006 as an assistant professor. Currently, he is a professor in the Department of Chemistry at IIT Kharagpur. His main area of research is the total synthesis of natural products and asymmetric synthesis with enzymes.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Chemistry in Molecular Flasks

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Indian Institute of Science
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Abstract:
Properties of chemical entities in confined nanospace are expected to be different from their bulk properties due to restricted movement. Such restricted degree of freedom along with other interaction/s may allow to stabilize unusual conformations of compounds in confined nanospace of molecular cavity. Unusual properties of photochromic spiropyrans in water soluble molecular barrels and stabilization of transient merocyanines in such molecular barrels will be discussed.[1-4] Our recent efforts on designing chiral molecular flasks including their chiral recognition will be discussed in my lecture. A recently developed strategy on constructing enantiopure cage (Figure 1) without using chiral donor/acceptor will be highlighted in the lecture.[5-7]

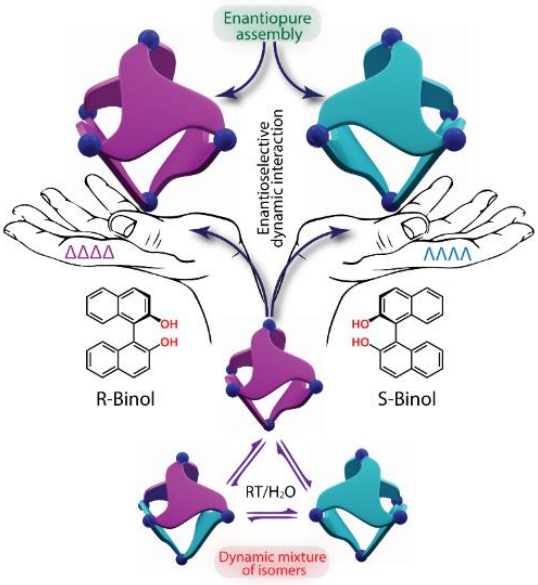


Figure 1 Guest induced enantiopure cage formation.

References and Notes:

1. Howladar, P.; Mondal, B.; Chowdhury, P.; Zangrando, E.; Mukherjee, P. S. *J. Am. Chem. Soc.* **2018**, *140*,7952.
2. Saha, R.; Devaraj, A.; Bhattacharyya, S.; Das, S.; Zangrando, E.; Mukherjee, P. S. *J. Am. Chem. Soc.* **2019**, *141*, 8638.
3. Saha, R.; Mondal, B.; Mukherjee, P. S. *Chem. Rev*. **2022**, *122*, ASAP.
4. Bhandari, P.; Modak, R.; Bhattacharyya, S.; Zangrando, E.; Mukherjee, P. S. *JACS-Au*, **2021**, *1*, 2242.
5. Arppitha, B. S.; Venkataswarulu, M.; Bhandari, P.; Clegg, J.; Mukherjee, P. S. *J. Am. Chem. Soc.* **2022**, *144*, 7504.
6. Howlader, P.; Zangrando, E.; Mukherjee, P. S. *J. Am. Chem. Soc.* **2020**, *142*, 9070.
7. Howlader, P.; Mondal, S.; Ahamed, S.; Mukherjee, P. S. *J. Am. Chem. Soc.* **2020**, *142*, 20968.

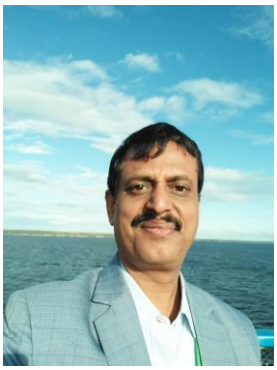
Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

Partha Sarathi Mukherjee



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Partha Sarathi Mukherjee worked under the supervision of Prof. N. Ray Chaudhuri at IACS (Kolkata) on Cu(II)-coordination polymers including their magnetic studies for his Ph.D. He was a postdoctoral fellow in the group of Prof. Peter Stang at the University of Utah and worked as an Alexander von Humboldt fellow at the University of Göttingen with Prof. Herbert Roesky before joining the Indian Institute of Science (IISc) as a faculty in 2005. Partha is currently a professor of chemistry at IISc (Bangalore).

He is a recipient of NASI-SCOPUS young scientist award, INSA-Medal, S. S. Bhatnagar prize, TWAS young affiliateship and Swarnajayanti fellowship of the Govt. of India. He was recently featured by the DST as one of the 75 scientists under 50 who are shaping the Indian science. He is an elected fellow of the Indian Academy of Sciences. Partha is/was in the editorial advisory boards of *Inorganic Chemistry*, *Inorganica Chimica Acta*, *Inorganic Chemistry Frontiers*, *The Chemical Records*, and *Scientific Reports*. He is currently serving as an Associate Editor of *Inorganic Chemistry*. He works on self-assembled discrete organic and coordination molecular architectures including their use in catalysis, sensing, and light-harvesting. He has published over 198 papers in peer-reviewed journals with a current *h-index* of 62.

Enantioselective Alkyl-Alkyl Coupling by Nickel Hydride Catalysis

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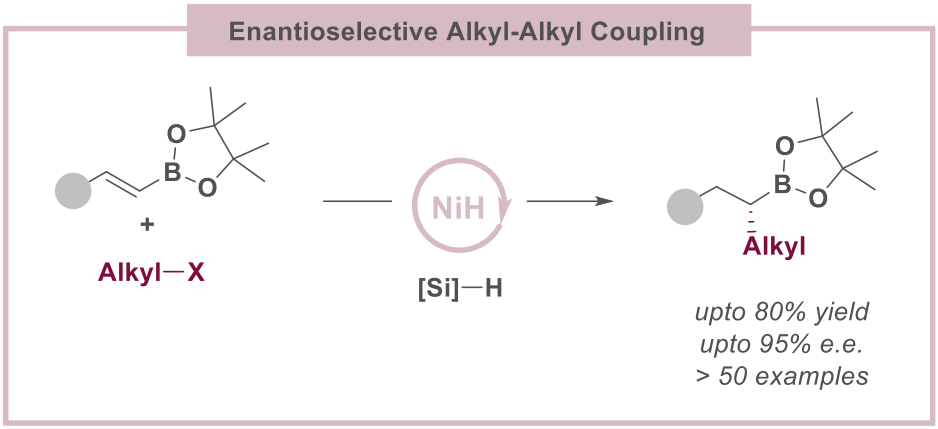
Abstract:
Recent analysis has suggested that molecules with a higher percentage of C(sp^3)-hybridized stereogenic centers have higher chances to succeed in clinical trials.[1] Transition metal-catalyzed enantioselective alkyl–alkyl coupling can generate such chiral 3D shape molecules.[2] This talk will demonstrate that the challenging enantioselective alkyl–alkyl coupling can be achieved by nickel hydride catalysis (Scheme).[3,4] The strategy enables enantioselective cross-coupling of non-activated alkyl halides with alkenyl boronates to produce chiral alkyl boronates. Employing readily available and stable olefins as pro-chiral nucleophiles, the coupling proceeds under mild conditions and exhibits broad scope and high functional group tolerance. Applications in the functionalization of natural products and drug molecules and the synthesis of chiral building blocks and a key intermediate to (*S*)-(+)-Pregabalin will be discussed.

Scheme:



References and Notes:

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2. Zhang, Z.; Bera, S.; Fan, C.; Hu, X. *J. Am. Chem. Soc*. **2022**, *144*, 7015 – 7029.
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4. Qian, Q.; Bera, S.; Hu, X. *J. Am. Chem. Soc.* **2021**, *143*, 1959 – 1967.

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Career Profile:
01/2022 – present: Assistant Professor of Organic Chemistry at Indian Institute of Technology Tirupati (IITT), India.
01/2018 – 12/2021: Postdoc with Prof. Xile Hu at EPFL, Switzerland.
Ph.D. (07/2017) in Organic Chemistry with Prof. Armido Studer at the University of Münster, Germany.
M.Sc. (2013) in Chemistry from IIT Kanpur (IITK), India. Supervisor: Prof. P. K. Bharadwaj.
B.Sc. (2011) in Chemistry (Honours) from R. K. Mission Residential College, Narendrapur (University of Calcutta), India.

Significant awards/achievements:
Postdoctoral fellowship by the SNSF, Switzerland (2018 – 2021).
Doctoral fellowship from the University of Münster, Germany (2013 –2017).
INSPIRE Scholarship from DST, India (2008 – 2013).
Dr. Shailendra Jha Memorial Prize in B.Sc. for 2nd highest marks in chemistry in 2011.
Scholarship of Merit in B.Sc. by the Indian Government (2008 – 2011).
AIR 3rd in IIT-JAM (Chemistry) in 2011.
2nd rank (with first-class) in B.Sc. at the University of Calcutta in 2011.
AIR 18th in GATE (Chemistry) in 2013.

Representative publications:
1. S. Bera, R. Mao, and X. Hu*, *Nat. Chem.* **2021**, *13*, 270–277.
2. S. Bera, and X. Hu*, *Angew. Chem. Int. Ed.* **2019**, *58*, 13854–13859.
3. S. Bera, C. G. Daniliuc and A. Studer*, *Angew. Chem. Int. Ed.* **2017**, *56*, 7402–7406.
4. S. Bera, C. G. Daniliuc, and A. Studer*, *Org. Lett.* **2015**, *17*, 4940-4943.
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6. Z. Zhang, S. Bera, C. Fan, and X. Hu*, *J. Am. Chem. Soc.* **2022**, *144*, 7015–7029
7. D. Qian, S. Bera, and X. Hu*, *J. Am. Chem. Soc.* **2021**, *143*, 1959–1967.

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Scientist: CSIR-Institute of Minerals and Materials Technology Bhubaneswar (2006) and continued to contribute to the affiliation since then.

Research domain: Molecular signaling in detection technology

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Human nature inspires precision engineering of proteins

Vishal Rai*
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Abstract:
The chemical toolbox for investigating biological systems or enabling biologics requires the precise covalent attachment of tags to the proteins. In this perspective, we have been leading the efforts toward chemical technologies to enable precise control over the site of bioconjugation. The critical barrier involves the simultaneous deconvolution of multiple challenges associated with reactivity and selectivity. In this perspective, we have developed a DisINtegrate or DIN theory that allows us to create new reactivity landscapes on a protein's surface. It enabled the development of methods for targeting reactivity hotspots,[1,2] N-Gly residue-specific labelling (Gly-Tag®),[3] and modular Linchpin-Directed Modification (LDM®) platform.[4] Our state-of-the-art platform offers homogeneous antibody-drug conjugates (ADCs) for directed cancer chemotherapeutics and fluorophore conjugates (AFCs) for imaging-guided tumour surgery.[4,5] Besides, our findings create a hope that we will make precision therapeutics with small molecules possible one day. *The talk would highlight the philosophical connection between humans and proteins' behaviour and how it inspired the precision engineering of proteins.*

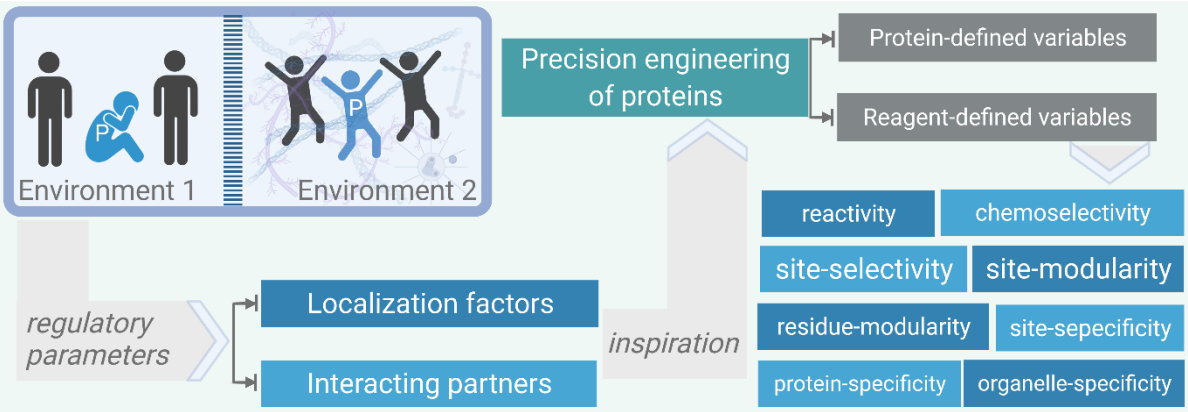

Figure: Regulatory parameters of human behavior inspired the precision engineering of proteins.

References and Notes:

1. For N-targeting, see: (a) *Chem. Commun.* **2015**, *51*, 473. (b) *Org. Biomol. Chem.* **2018**, *16*, 9377. (c) *Chem. Commun.* **2021**, *57*, 7083.
2. For reactivity hotspots, see: (a) *Chem. Commun.* **2019**, *55*, 1100. (b) *Chem. Commun.* **2018**, *54*, 7302. (c) *Chem. Eur. J.* **2017**, *23*, 3819. (d) *Chem. Commun.* **2017**, *53*, 959.
3. Gly-Tag®: (a) *Nat. Commun.* **2019**, *10*, 2539. (b) *Chem. Sci.* **2020**, *11*, 13137.
4. LDM® platform and ADCs: (a) *J. Am. Chem. Soc.* **2018**, *140*, 15114. (b) *Angew. Chem. Int. Ed.* **2020**, *59*, 10332. (c) *Chem. Sci.* **2021**, *12*, 6732. (d) *Chem. Commun.* **2022**, *58*, 1768.
5. Our other ADCs: (a) *Nat. Biomed. Eng.* **2019**, *3*, 917. (b) *Chem. Commun.* **2019**, *55*, 9979.

Bio-Sketch of Speaker

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Dr. Vishal Rai obtained his Ph.D. in Chemistry from IIT Bombay (2003-2008). He subsequently held a postdoctoral position and MITACS-Elevate fellow position at the University of Toronto, Canada (2008-2011). His contributions to peptide macrocycles created the platform for Encycle Therapeutics. Later, he joined the Department of Chemistry at IISER Bhopal in 2011.

Positions, Awards, and Honours: He is the Founder and Director of *Plabeltech Private Limited*. The state-of-the-art protein and antibody engineering technologies such as LDM®, Gly-Tag®, and Maspecter® empower the company. Recently, his team established the Precision Antibody Engineering CEnter (*SERB-PACE*) to meet India's technological demands in biologics. Also, he is the recipient of the Swarnajayanti Fellowship, Ramanujan Fellowship, CRSI Bronze Medal, CDRI Award for excellence in drug research, SERB Technology Translation Award, RSC-WIS Young Scientist Award, and DAE Young Scientist Award. Recently, he joined the *ACS Chemical Biology* team as an Early Career Board member. He has been involved in scientific outreach activities as national co-chair (India) for the International Chemical Biology Society (ICBS). Also, he is an invited Fellow of the Royal Society of Chemistry (FRSC), UK.

Research interests: His research group is leading the development of chemical technologies for the *precision engineering of proteins*. They are also involved in synthesizing homogeneous antibody-conjugates, protein immobilization, and analytical tools for peptides and proteins. His research team wants to contribute to Society through homogeneous bioconjugates for directed cancer chemotherapeutics and surgical oncology. Besides, they are investing efforts to make small-molecule precision therapeutics possible in the future.

Hydrosilylation of Activated Alkenes Enabled through Photoinduced Hydrogen Atom Transfer Catalyst

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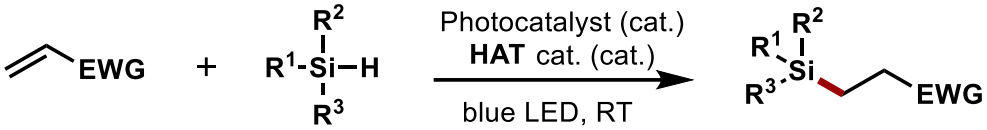
Abstract:

Organosilanes are versatile synthon in the field of organic chemistry and they have widespread applications in material science, agrochemicals, and polymer science.[1] Because of the high lipophilicity nature of silicon, organosilanes and silyl analogs of bioactive molecules exhibits remarkable physiochemical properties which makes them an ideal candidate for medicinal chemistry.[2] Hydrosilylation of alkene using hydrosilanes represents one of the most atom economical approach for the synthesis of Organosilanes.[3]



Scheme 1: Photocatalytic hydrosilylation of electron deficient alkenes with silanes

Past decade has witnessed the significant renaissance of visible light photocatalysis in the field of synthetic organic chemistry. In addition to single electron transfer (SET) and energy transfer, hydrogen atom transfer (HAT) is more frequently encountered in photocatalysis. Recent efforts on selective Si-H functionalization of hydrosilanes under photolytic conditions suffers from site poor selectivity[4] due to the similar BDEs (C-H vs Si-H).[5]

In this presentation, new design and synthetic utility of Hydrogen atom transfer catalyst for the visible light mediated photoredox catalytic hydrosilylation of activated alkenes using hydrosilanes as silyl radical precursor will be discussed.

References and Notes:

1. (a) Mizoshita, N.; Tani, T.; Inagaki, S. *Chem. Soc. Rev*. **2011**, *40*, 789; (b) Dang, T. T.; Nguyen, H. M. T.; Nguyen, H.; Dung, T. N.; Nguyen, M. T.; Dehaen, W. *Molecules* **2020**, *25*, 548.
2. For selected reviews, please see: (a) Pooni, P. K.; Showell, G. A. *Mini-Rev. Med. Chem*. **2006**, *6*, 1169; (b) Franz, A. K.; Wilson, S. O. *J. Med. Chem*. **2013**, *56*, 388; (c) Taylor, R. D.; MacCoss, M.; Lawson, A. D. G. *J. Med. Chem*. **2014**, *57*, 5845; (d) Ramesh, R.; Reddy, D. S. *J. Med. Chem*. **2018**, *61*, 3779.
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Selvakumar was born and grew up in Tindivanam, Tamilnadu, India. After his post graduation from University of Madras, he moved to IIT Kanpur in 2004 to pursue his doctoral research in the group of Professor Vinod K. Singh in the area of enantioselective C-C bond forming reactions. After completing his Ph.D. in 2009, he started his postdoctoral research at the North Dakota State University, USA with Professor Mukund P. Sibi where he worked in the area of enantioselective organocatalytic photocycloaddition reactions and biomass conversion to value added chemicals. In November 2013, he moved to Kyoto University, Japan to join the research group of Professor Keiji Maruoka to work on Hypervalent iodine reagent mediated C-H bond activation and asymmetric organocatalytic biomimetic transamination reaction. In November 2017 he was appointed as a UGC-Assistant Professor at the Central University of Haryana, India. Since September 2019 he is holding a position of Assistant Professor at Indian Institute of Technology Indore, India. His current research focussed on the development of sustainable photochemical methods and Asymmetric synthesis.

Bio-Sketch of Speaker

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Dr. Anand Singh graduated with M.Sc. degree in Organic Chemistry from IIT Bombay in 2004. Subsequently, he obtained Ph.D. in synthetic organic chemistry from Vanderbilt University in 2009. He held a postdoctoral position at the Sanford-Burnham Medical Research Institute until 2013. He subsequently joined IIT Kanpur in 2013 and is now an Associate Professor in the Department of Chemistry. His research interests include visible light photocatalysis, synthetic methodologies toward fluorinated molecules and heterocycles, radical mediated organic transformations, and materials for solar photovoltaics.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Halogen–Bonding Catalysis for Organic Synthesis

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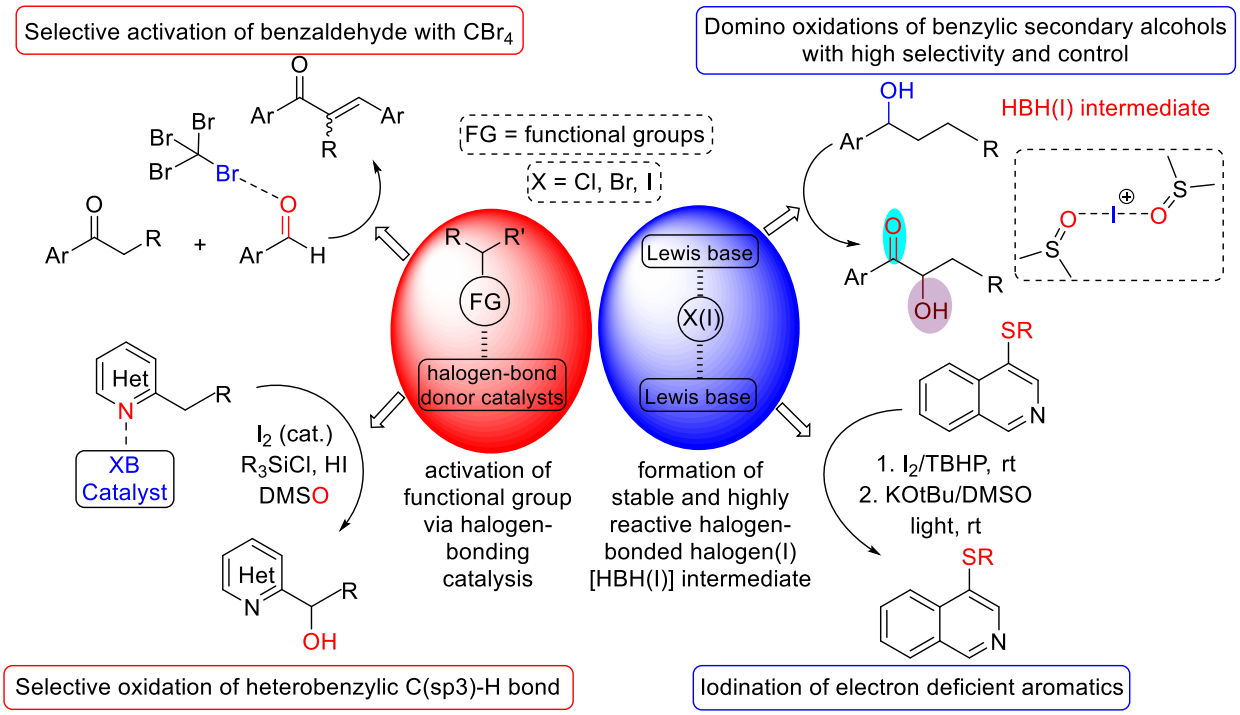
In recent years, halogen bond donor organocatalysts have been employed to activate the Lewis basic functional groups.[1,2] The halogen–bonding (XB) interaction between the Lewis bases and the halogen(I) reagents or intermediates (halonium ions) is shown to enhance the reactivity and selectivity.[2b] Recently, we have developed new iodine(I) and iodine(III) halogen bond donor catalysts for transition metal-free organic reactions where halogen–bonded halogen species act as key intermediates with unusual reactivity and selectivity (Figure 1).[2] For example, CBr_4 has been employed as a recoverable halogen bond donor catalyst for selective activation of aldehydes to synthesize *α,β*–unsaturated ketones.[2a] NBS and *in situ*–generated acetyl hypoiodite (CH_3COOI) have been employed for selective oxidation of heterobenzylic C(sp^3)–H bond to C(sp^2)–O and C(sp^3)–O bonds *via* activation of the heterocyclic ring.[2b] The halogen–bonded iodonium ions have been utilized as stable and key oxidants to develop domino oxidation of benzylic secondary alcohols with high selectivity to synthesize α–hydroxy ketones.[3] Also, we have developed an iodination and thioether formation for electron-deficient aromatic rings under mild conditions.[3]



References and Notes:

1. Cavallo, G.; Metrangolo, P.; Milani, R.; Pilati, T.; Priimagi, A.; Resnati, G.; Terraneo, G. *Chem. Rev.* **2016**, *116*, 2478.
2. (a) Bulfield, D.; Huber, S. M. *Chem. Eur. J.* **2016**, *22*, 14434. (b) Guha, S.; Kazi, I.; Nandy, A.; Sekar, G. *Eur. J. Org. Chem.* **2017**, *23*, 5497.
3. (a) Kazi, I.; Guha, S.; Sekar, G. *Org. Lett.* **2017**, *19*, 1244. (b) Guha, S.; Kazi, I.; Mukherjee, P.; Sekar, G. *Chem. Commun.*, **2017**, *53*, 10942. (c) Guha, S.; Sekar, G., *Chem. Eur. J.* **2018**, *24*, 14171. (d) Guha, S.; Kazi, I.; Sathish, D.; Sekar, G. *J. Org. Chem.* **2022**, *87*, 5424.

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Prof. G. Sekar obtained his Ph.D. from IIT Kanpur in 1999 under the guidance of Padma Shri, Prof. Vinod K. Singh. Sekar was a JSPS postdoctoral fellow at TUT Japan, and an AvH postdoctoral fellow at Goettingen University, Germany. He also carried out postdoctoral research at Caltech, USA.

He is the recipient of the Senior Scientist Award-2021 by the Academy of Sciences Chennai, CRSI bronze medal-2015, and Institute Research and Development Award (Mid-Career)-2017. He is a Fellow National Academy of Sciences (2019), a Fellow of the Royal Society of Chemistry, and a Fellow of the Academy of Sciences, Chennai. He is a council member of the NOST, CRSI, and the Academy of Sciences, Chennai.

Prof. Sekar's research activity on organic synthesis focuses on developing new synthetic methodologies employing environmentally benign homogeneous catalysts, metal nanocatalysts, and halogen bonding catalysis.

Sustainable Catalyst Designing for Renewable Hydrogen Production and Small Molecule Activation

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Abstract:

The replacement of hazardous and waste-generating reagents and precursors with "greener" and "renewable" alternatives is a significant task where organometallic catalysis is the key technology to convert challenging substrates to useful chemicals.[1]
Major attention requires to their energy efficiency, cost-effectiveness, and environmental aspects. To reduce carbon emissions and global warming effects, the demand for sustainable and clean energy has now become more significant. Hydrogen is considered the ideal energy source of the future if it can be generated from renewable resources efficiently and sustainably. Application of (de)hydrogenation reactions to convert waste to useful chemical resources is part of the circular economy where hydrogen can be produced as the major by-product.[2] Currently ~95% of hydrogen gas was produced from fossil fuels, mainly via steam reforming of natural gas, resulting in dependence on fossil fuels. To overcome these limitations, biomass derivatives presents as a potential renewable feedstock for H_2 production.
The new generation of sustainable, robust catalyst development opens up a new avenue for renewable H_2 production. Simultaneously the particular catalyst design also actively participates in the small molecule activation chemistry to produce the value-added chemicals via a greener reaction pathway.[3]

References and Notes:

1. Homogeneous first-row transition metal catalyst for sustainable hydrogen production and organic transformation from methanol, formic acid, and bio-alcohols, J. Rana, S. T. Sahoo, Prosenjit Daw*, *Tetrahedron* **2021**, 132473.
2. Homogeneous Catalysis for Sustainable Energy: Hydrogen and Methanol Economies, Fuels from Biomass, and Related Topics, A. Kumar*, Prosenjit Daw*, David Milstein*, *Chem. Rev.* **2022**, *122*, 385-441.
3. Application of pincer metal complexes in catalytic transformations, A. Mohanty, R. Sharma, Prosenjit Daw*, *Pincer-Metal Complexes.* **2022**, 1-68. (Book chapter)

Bio-Sketch of Speaker

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Career Profile:

- Assistant Professor: Department of Chemical Sciences, Indian Institute of Science Education and Research, Berhampur, India, September 2019 - Present
- Post-Doctoral: Weizmann Institute of Science, Israel, Advisor: Prof. David Milstein, 2015-2019
- Ph.D: Indian Institute of Technology Kanpur, Kanpur, India, Advisor: Prof. Jitendra K. Bera, 2009-2015
- M.Sc: Indian Institute of Technology Kanpur, Kanpur, India, Advisor: Prof. Jitendra K. Bera, 2007-2009

Awards/achievements

- 11th CaRLa Winter School, 2018 on Homogeneous Catalysis, organized by BASF and University of Heidelberg, Heidelberg, Germany. 18-23 February 2018. (Oral & poster presentation). 2nd Best Poster award
- Shyama Prasad Mukherjee Fellowship (SPMF), 2009, in chemical science by Council of Scientific & Industrial Research (CSIR), New Delhi, India.
- Senior Postdoctoral fellowship of Weizmann Institute of Science, Israel, (2018-2019)
- Planning and Budgeting Committee (PBC) fellowship of the Council for Higher Education, Israel. (2015-2018)

Representative publications:

1. Homogeneous Catalysis for Sustainable Energy: Hydrogen and Methanol Economies, Fuels from Biomass, and Related Topics, A. Kumar*, **Prosenjit Daw***, David Milstein*, Chem. Rev. 2022, 122, 385-441.
2. Application of pincer metal complexes in catalytic transformations, A. Mohanty, R. Sharma, **Prosenjit Daw***, Pincer-Metal Complexe. 2022, 1-68. (Book chapter)
3. Homogeneous first-row transition metal catalyst for sustainable hydrogen production and organic transformation from methanol, formic acid, and bio-alcohols, J. Rana, S. T. Sahoo, **Prosenjit Daw***, Tetrahedron 2021, 132473.
4. Direct Synthesis of Amides by Acceptorless Dehydrogenative Coupling of Benzyl Alcohols and Ammonia Catalyzed by a Manganese Pincer Complex: Unexpected Crucial Role of Base, **Prosenjit Daw**, A Kumar, NA Espinosa-Jalapa, Y Ben-David, D Milstein*, J. Am. Chem. Soc. 2019, 141, 12202-12206.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

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: RC tripathi award by Orissa chemical society

Selected publications

1. RSC Advances (2015), 5(91), 74457-74462.
2. ChemistrySelect (2017), 2(33), 10699-10703
3. CrystEngComm (2017), 19(32), 4759-4765.
4. ChemistrySelect (2016), 1(8), 1630-1635.

Covalent Organic Frameworks as Platform for Charge-storage

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Abstract: Covalent Organic Framework (COF) as crystalline organic polymer has rapidly surged since 2005. The modular framework of COF offers room for by-design functional manipulation in an application-specific manner. Their lightweight nature, high surface area, and processability have signified them as a potential candidate for many charge-storage systems. Large micro-mesopores favor rapid diffusion of charged ions, which is guided by the intrinsic electronics of the conjugated framework. Unfortunately, in many cases, due to the inherent defects in the framework, the conjugation does not propagate sufficiently, leading to poor conductivity. To substitute this, conducting carbons are typically added to boost their conductivity, enhancing their charge storage properties. Here we embrace a different approach to achieving this. Our versatile strategy yields a carbon-free conducting COF displaying substantially high energy and power density in a supercapacitor configuration. This presentation will brief our approach and findings.

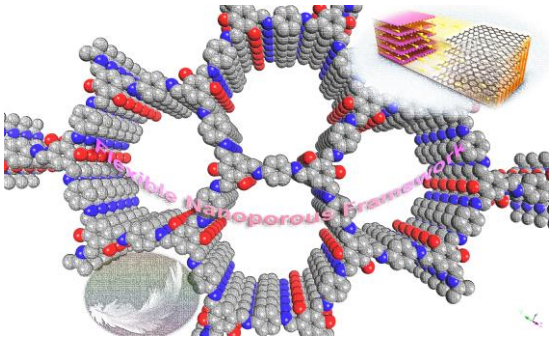

Figure 1. COF for lightweight rapid charge-discharge storage

References and Notes:

(i) Covalent Organic Frameworks for Batteries, Zhu et al., *Adv. Funct. Mater.* 31, 2100505 (2021); (2) 2D Covalent Organic Framework Electrodes for Supercapacitors and Rechargeable Metal-Ion Batteries, Kandambeth et al., *Advanced Energy Materials*, 12, 4, (2021); (3) Exceptional Capacitance Enhancement of a Non-Conducting COF through Potential-Driven Chemical Modulation by Redox Electrolyte, Kushwaha et al., *Adv. Energy Mater.*, 1, 2003626 (2021); (4) Tuning the electronic energy level of covalent organic frameworks for crafting high-rate Na-ion battery anode, Haldar et al., *Nanoscale Horiz.*, 2020, 5, 1264-1273 (2020).

Bio-Sketch of Speaker

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Dr. R. Vaidhyanathan obtained his Ph.D. from the Jawaharlal Nehru Centre for Advanced Scientific Research under Prof. C. N. R. Rao and Prof. S. Natarajan. He worked as a postdoc with Prof. M. J. Rosseinsky at the University of Liverpool and as a research associate with Prof. George Shimizu at the University of Calgary. He started his independent research career as an assistant professor in IISER Pune in 2012. Currently, he is an Associate Professor at IISER Pune. His research focuses on developing Advanced Porous Materials such as metal-organic frameworks (MOFs) and covalent-organic frameworks (COFs) and their nanocomposites for environmental and energy applications. He has published over 101 papers and has 11 patents filed from IISER Pune. He has been rewarded with several honors, including the C.N.R. Rao Award. National Prize for research in Physical and Inorganic Chemistry (2021), Materials Research Society of India Medal (2019), Chemical Research Society of India Medal (2018), IUSSTF funding won jointly with Temple University (Chief Co-PI, 2018), Sakurai Science Program (SSP), Osaka University, Japan (2016), Best Emerging Young Scientist (Chemical Frontiers), Goa, (2017). He serves as an Editorial Board Member of ACS Materials Letters and Nature Scientific Reports. He is an Associate Editor of ACS Chemistry of Materials.

Relevant publications:

1. Exceptional Capacitance Enhancement of a Non-Conducting COF through Potential-Driven Chemical Modulation by Redox Electrolyte, Kushwaha R, Haldar S, Shekhar P, Krishnan A, Jayeeta S, Hui P, Vinod CP, Subramaniam C, Vaidhyanathan R, *Adv. Energy Mater.*, 11, 2003626 (2021).
2. Facile Exfoliation of Single-Crystalline Copper Alkylphosphates to Single-Layer Nanosheets and Enhanced Supercapacitance, Bhat GA, Haldar S, Verma S, Chakraborty D, Vaidhyanathan R, Murugavel R, *Angew. Chem. Int. Ed.*, 58,16844–16849 (2019).
3. Tuning the electronic energy level of covalent organic frameworks for crafting high-rate Na-ion battery anode, Haldar S, Kaleeswaran D, Rase D, Roy K, Ogale S, Vaidhyanathan R, *Nanoscale Horiz.*, 5, 1264-1273 (2020).
4. Chemical Exfoliation as a Controlled Route to Enhance the Anodic Performance of COF in LIB, Haldar S, Roy K, Kushwaha R, Ogale S, Vaidhyanathan R, *Adv. Energy. Mater.*, 9, 1902428 (2019).
5. Pyridine-Rich Covalent Organic Frameworks as High-Performance Solid-State Supercapacitors, Haldar S, Kushwaha R, Maity R, Vaidhyanathan R, *ACS Materials Lett.*, 4, 490–497 (2019).
6. High and Reversible Lithium Ion Storage in Self-Exfoliated Triazole-Triformyl Phloroglucinol based Covalent Organic Nanosheets, Haldar S, Roy K, Nandi S, Chakraborty D, Puthusseri D, Gawli Y, Ogale S, Vaidhyanathan R, *Adv. Energy Mater.*, 8, 1702170 (2018).

Merger of Photoredox-/Electro-catalysis with Organocatalysis: A Sustainable Approach Towards the Asymmetric Synthesis of Dihydrodibenzo-oxazepines

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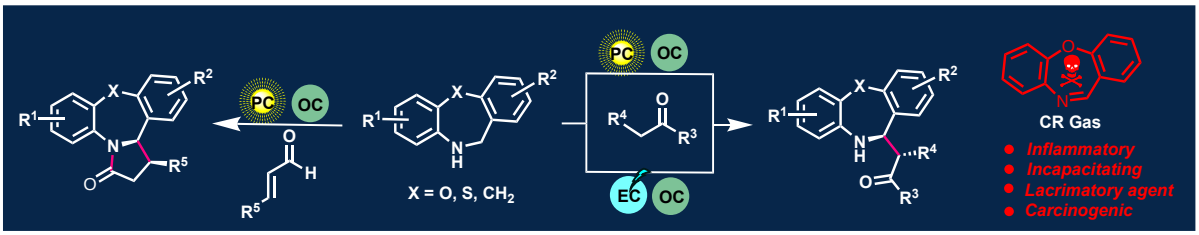
Abstract:
Since the renaissance of organocatalysis and photo-redox catalysis, both areas individually have enjoyed immense success in developing new and challenging organic transformations, even in the highly stereoselective fashions. The merger of visible light catalysis with asymmetric organocatalysis has turned out as an effective strategy that has successfully been applied for the α-functionalization of carbonyl compounds and amines. Recently, organocatalysts have shown excellent compatibility with electrocatalysis to carry out challenging asymmetric transformations, which seem difficult to realize in the absence of either of the catalytic systems. Undoubtedly, the applications of organo-, photoredox- and electrocatalysis offer manifold advantages, which could lead to the development of new organic transformations and solve practical problems associated with organic synthesis. One such practical and the operational problem is associated with the synthesis of dihydrodibenzo[b,f][1,4]oxazepine - an important class of *N*-heterocycles featured in drugs and bioactive compounds.[1] Due to attractive biological activities, the already developed enantioselective syntheses of oxazepine derivatives relies on the nucleophilic addition to the C=N of the dibenzoxazepines *i.e.*, CR gas.[2] This structural unit is the primary riot-controlling agent in tear gas, and it can cause severe health issues by being carcinogenic, incapacitating, inflammatory, and lacrimatory agents.[3] CR gas can also cause temporary blindness, cough, shortness of breath, panic, and blepharospasm. The excess inhalation may cause even death due to asphyxiation and pulmonary edema.

With the hazardous effects of CR Gas in view, developing an alternate strategy to avoid its direct use is highly desirable. Therefore, we envisioned that the dibenzoxazepine unit could be generated *in-situ* from the corresponding user-friendly oxazepine, either *via* photoredox or electrochemical oxidation. Subsequently, the *in-situ* generated dibenzoxazepine will be trapped with an organocatalytically generated nucleophile to form a new carbon-carbon bond in a highly stereoselective manner. In this context, we have merged proline-catalysis with photoredox- or electrocatalysis to undergo a highly stereoselective oxidative Mannich reaction.[4] Further, a merger of NHC catalysis with photoredox catalysis to undergo oxidative annulation reactions is currently being developed in our lab.[5] Key results of our findings on the combination of chiral organocatalysis with photoredox-/electrocatalysis will be presented.



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1. (a) R. Li, P. S. Farmer, J. Wang, R. J. Boyd, T. S. Cameron, M. A. Quilliam, J. A. Walter, S. E. Howlett, *Drug Des. Discov.* **1995**, *12*, 337-358; (b) S. M. Lynch, L. Tafesse, K. Carlin, P. Ghatak, D. J. Kyle, *Bioorg. Med. Chem. Lett*. **2015**, *25*, 43-47.
2. L. D. Munck, C. Vila, J. R. Pedro, *Eur. J. Org. Chem*., **2018**, 140-146.
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5. Y. Hussian, P. Chauhan, *Under preparation.*

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

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Position Held:

- **Assistant Professor** at IIT Jammu (October 2017-till date)
- **Sub Group Leader** with Prof. Dieter Enders at RWTH Aachen University, Germany (April 2014-September 2017).
- **Postdoctoral Researcher** with Prof. Dieter Enders at RWTH Aachen University, Germany (April 2013-March 2014).
- **Research Associate** with Prof. Swapandeep Singh Chimni at Guru Nanak Dev University, Amritsar, India (November 2012-March 2013).

Education:

- Ph.D. from Guru Nanak Dev University, India (Ph. D. Supervisor - Prof. Swapandeep Singh Chimni, Ph.D. date: 29th November 2012). Thesis Title - **Enantioselective Carbon-Carbon Bond Formation Catalyzed by Cinchona-Derived Organocatalysts**.
- M.Sc. Chemistry from Guru Nanak Dev University, India (2007).
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Scholarships and Awards:

- RSC Research Fund (2022)
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- Selected for "Research in Paris" France (2013, declined).
- Selected for "Science without Border" Brazil (2013, declined).
- International Travel Grant by DST India (2011).

Representative publications:

1. Tamanna, Y. Hussian, D. Sharma, **P. Chauhan*** Asymmetric Synthesis of Cyclohexenone Fused Isochromans via Quinidine Catalyzed Domino Peroxyhemiacetalization/Oxa-Michael Addition Desymmetrization Sequence, *J. Org. Chem.* **2022**, https://doi.org/10.1021/acs.joc.2c00215.
2. Y. Hussian, D. Sharma, N. Kotwal, I. Kumar, **P. Chauhan***, Stereoselective Oxidative Mannich Reaction of Ketones with Dihydrodibenzo-oxazepines *via* a Merger of Photoredox-/Electro-catalysis with Organocatalysis. *ChemSusChem.* **2022**, https://doi.org/10.1002/cssc.202200415.
3. Y. Hussian, Tamanna, M. Sharma, A. Kumar, **P. Chauhan***, Recent Development in Asymmetric Organocatalytic Domino Reactions Involving 1,6-Addition as a Key Step, *Org. Chem. Front.,* **2022**, 9, 572-592.
4. Tamanna, M. Kumar, K. Joshi, **P. Chauhan***, Catalytic Asymmetric Synthesis of Isochroman Derivatives, *Adv. Synth. Catal.* **2020**, *362*, 1907-1926.
5. **P. Chauhan***, N-Heterocyclic carbene catalysed umpolung reactions of imines approaching enantioselective synthesis, *Org. Chem. Front.,* **2019**, *6*, 3821-3824.
6. U. Kaya, **P. Chauhan***, S. Mahajan, K. Deckers, A. Valkonen, K. Rissanen and D. Enders, Asymmetric Squaramide Catalyzed Domino aza-Friedel-Crafts/N,O-Acetalization Reactions Between Naphthols and Pyrazolinone Ketimines, *Angew. Chem. Int. Ed.* **2017**, *56*, 15358-15362 (**Highlighted in Synfacts**).

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Amlan Kusum Roy

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Amlan. K. Roy completed his PhD in theoretical chemistry from Panjab University, in India. Later he pursued his post-doctoral research in a number of places in North America, such as University of New Brunswick (Fredericton, Canada), University of Kansas (Lawrence, USA), University of California (Los Angeles, USA), University of Florida (Quantum Theory Project). His primary research interest is to develop methods for electronic structure and dynamics of many electron systems, within the broad domain of density functional framework. Presently he is a professor at IISER Kolkata. He has published about ninety research papers and book chapters in reputed journals. He has been serving as a reviewer in several renowned journals. His biography has been included in 63rd Edition of Marquis Who's Who in America, 2009. In 2012, he has edited a book entitled "Theoretical and Computational Developments in Modern Density Functional Theory".

Selected Publications :

1. A. Ghosal and **A. K. Roy,** A real-time TDDFT scheme for strong-field interaction in Cartesian coordinate grid, *Chem. Phys. Lett.* **796,** 139562 (2022).
2. R. Roy, A. Ghosal and **A. K. Roy,** Charge-transfer excitation within a hybrid-(G)KS framework through Cartesian grid DFT, *J. Phys. Chem. A* **126,** 1448 (2022).
3. N. Mukherjee and A. K. Roy, Multipole oscillator strength and polarizability for confined hydrogen-like atoms under high pressure, *J. Phys. B* **55**, 145001, (2022).
4. N. Mukherjee and **A. K. Roy,** Shell-confined atom and plasma: incidental degeneracy, metallic character, and information entropy *Phys. Rev. A* **104,** 042803 (2021).
5. A. Ghosal and **A. K. Roy** A self-consistent systematic optimization of range separated hybrid functionals from first principles, *Mol. Phys.* e1983056 (2021).
6. N. Mukherjee, C. N. Patra and **A. K. Roy,** Confined hydrogenlike ions in plasma environments *Phys. Rev. A* **104,** 012803 (2021).
7. S. Majumdar and **A. K. Roy,** Density functional study of atoms spatially confined inside a hard sphere, *Int. J. Quant. Chem.* **121,** e26630 (2021).
8. Sangita Majumdar, Neetik Mukherjee and **Amlan K. Roy,** Information entropy and complexity measure in generalized Kratzer potential, *Chem. Phys. Lett.* **716,** 257-264 (2019).
9. N. Mukherjee and **A. K. Roy,** Quantum mechanical virial-theorem for confined quantum systems, *Phys. Rev. A* **99,** 022123-11 (2019).

Helical Scaffolds for Selective Charge Transfer Interactions and Efficient Proton Conduction

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Abstract:
Organic molecules offer structural diversity, established protocols of synthesis, good thermal stability, and low density, making them highly attractive as photoactive materials and for proton conductivity. This talk will describe our efforts towards employing conformationally-rigid helical scaffolds based on pyridine-2,6-dicarboxamide residue towards for:

(i) imparting high selectivity in intermolecular charge transfer interactions resulting in prominent organizational and morphological changes in the self-assemblies
(ii) significantly enhancing solid-state proton conductivity of discrete uncharged organic molecules with the efficiency of proton conduction for the homochiral self-assemblies outperforming those for the heterochiral self-assemblies.

These exciting outcomes will be presented in detail during the talk.

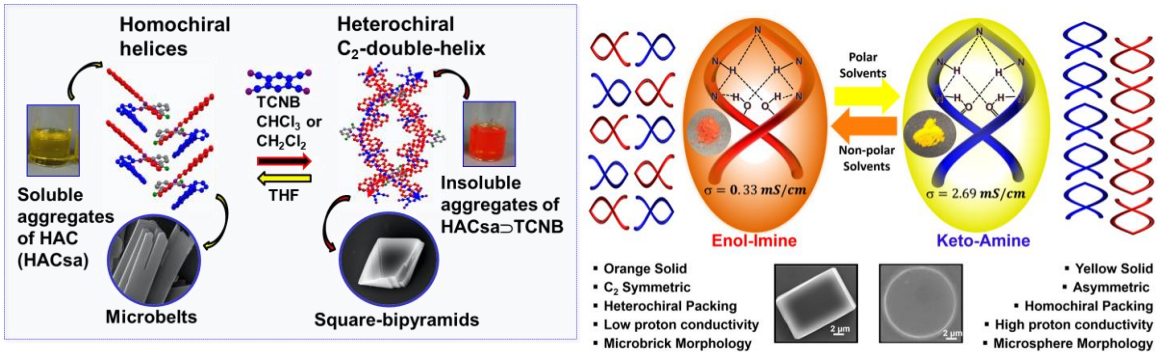

Figure 1: Left: Electron-rich residues appended to helical scaffolds elicited selective charge transfer interactions with electron-deficient guests. Right: Stereo-divergent self-assemblies of tautomerizable residues appended to helical scaffolds showed varied morphology and proton conductivity.

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2. Kumar, R.; Aggarwal, H.; Bhowal, R.; Chopra, D.; Srivastava, A. *Chemistry–A European Journal* **2019**, *25* (45), 10756–10762.
3. Kumar, R.; Aggarwal, H.; Srivastava, A. *Chemistry–A European Journal* **2020**, *26* (47), 10653–10675
4. Aggarwal, H.; Gaikwad, P. A.; Dahat, A.; Ghosh, S. N.; Talukder, S.; Srivastava, A. *manuscript under preparation*

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Dr. Aasheesh Srivastava is Professor at the Department of Chemistry, IISER Bhopal. He joined IISER Bhopal as Assistant Professor in late 2009 and became Associate Professor in 2015. His research interests lie at the interface of Chemistry, Materials and Biology. His group undertakes chemical synthesis of biodegradable polymers and low molecular weight hydrogelators for drug delivery and antimicrobial/ antifouling coating applications. He has also designed multi-responsive photoactive scaffolds and explored benign protocols for preparing nanomaterials for energy applications. He is an Advisory Board Member of the journal *Biomaterials Science* published by the Royal Society of Chemistry. He has coauthored more than 50 scientific publications and has filed 2 patent applications. He was the Head of the Department from July 2017-Dec 2019. He has guided 08 students for their PhD, and 13 students for their MS thesis.

Dr. Srivastava had his early education in New Delhi and obtained B.Sc. (Honours) Chemistry in 1997 from University of Delhi. He subsequently moved to IIT Kanpur for his M.Sc. in Chemistry (completed in 1999), which was followed by a PhD from the Indian Institute of Science, Bangalore. He was a postdoctoral researcher position at the Materials Research Laboratory of the University of California at Santa Barbara (UCSB) between 2006-2009 where he researched on Bioinspired Materials.

Deciphering the chemo-mechanical coupling mechanisms of ATP-dependent enzymes using single-molecule force spectroscopy

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Abstract:
Energy-dependent enzymes perform many key cellular processes such as protein degradation and disaggregation and act as biological molecular motors converting chemical energy from hydrolysis of ATP to mechanical energy. These enzymes utilize this energy to perform activities such as protein unfolding and translocation that are essential during many cellular processes. Although the biochemical mechanisms of these enzymes are well-understood, the biophysical properties such as kinetics, translocation velocities, and the stepping dynamics, as well as the energetic costs of these individual mechanical processes have not been studied in detail. Single-molecule force spectroscopic tools such as optical tweezers have enhanced our understanding of protein mechanics and the mechanism of action of molecular motors by complementing the bulk biochemical/biophysical methods. Single-molecule measurements allow examination of individual processes of a multi-step reaction as well as highlight the heterogeneity in their molecular properties that are masked in bulk averaging.

In the current talk, I will discuss my recent research on the application of optical tweezers to understand the role of protein substrate directionality on protein degradation by an ATP-dependent protease, ClpAP. Our results highlight the paramount role of local stability in protein degradation and provide clues as to how the placement of degradation signals on a substrate may evolve to minimize the energetic cost of degradation[1]. Continuing on the mechanism of ClpAP, we have deciphered the role of individual ATPase motors in a double-ring ATPase enzyme, ClpAP[2]. Further, I will elaborate on my current research projects on the application of optical tweezers and spectroscopic techniques to elucidate the mechanism of protein degradation by *Mycobacterium Tuberculosis* proteasomal complex.

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* Equal contribution.
[2] Kotamarthi, H.C.; Sauer, R.T.; Baker, T.A. *Cell Reports.* **2020,** *30*, 2644-2654.

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

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Career Profile:

Assistant Professor, Department of Chemistry, IIT- Madras.
Postdoctoral Researcher, Department of Biology, Massachusetts Institute of Technology.
Graduate student, Department of Chemical Sciences, TIFR, Mumbai.

Significant awards/achievements:

- Education committee travel award for attending 61st Biophysical society meeting, 2017, U.S.A.
- Honorable mention for the best thesis award in chemistry at TIFR during 2014-2015.
- Student Research Achievement Award for the best poster in Mechanobiology subgroup at 58th Biophysical Society, USA, 2014.

Representative publications:

1. Gokul Nalupurackal, Gunaseelan M., Muruga Lokesh, Rahul Vaippully, Amit Chauhan, B. R. K. Nanda, Chandran Sudakar, **Hema Chandra Kotamarthi**, Anita Jannasch, Erik Schaffer, Jayaraman Senthilselvan, and Basudev Roy. "Simultaneous optical trapping and magnetic micromanipulation of ferromagnetic iron-doped upconversion microparticles in six degrees of freedom" (Submitted)
2. **Hema Chandra Kotamarthi,** Robert Sauer, Tania Baker. "The non-dominant AAA+ ring in the ClpAP protease functions as an anti-stalling motor to accelerate protein unfolding and translocation", **Cell Reports**, 2020, Vol 30, 2644-2654.
3. Adrian Olivares*, **Hema Chandra Kotamarthi***, Benjamin Stein, Robert Sauer, Tania Baker, "Effect of directional pulling on mechanical protein degradation by ATP-dependent proteolytic machines", ***Proceedings of National Academy of Sciences***, *USA*, 2017, Vol 114, E6306-E6313. * Equal Contribution.
4. **Hema Chandra Kotamarthi,** Riddhi Sharma, Satya Narayan, Sayoni Ray, and Sri Rama Koti Ainavarapu. "Multiple unfolding pathways of leucine binding protein (LBP) probed by single- molecule force spectroscopy (SMFS)", ***Journal of the American Chemical Society***, 2013, Vol 135, 14768-14774.

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Amit Paul received his B.Sc. from Jadavpur University, M.Sc. from IIT Bombay, and Ph.D from the University of Pittsburgh with Prof. David H. Waldeck in 2008. He was then a postdoctoral research associate as a part of the Energy Frontier Research Center (EFRC) at the University of North Carolina at Chapel Hill with Prof. Thomas. J. Meyer. In October, 2011, he joined the Indian Institute of Science Education and Research (IISER) Bhopal as an Assistant Professor and was subsequently promoted to an Associate Professor in August, 2018. He was awarded as DAE young scientist in 2013. He was highlighted as New Frontiers in Indian Research by RSC in 2017 and Emerging Investigator by Chemical Communications, RSC in 2018. His group is interested in electrochemical applications of electrochemical supercapacitor, heterogeneous water oxidation, electro-organic synthesis etc.

Selected Publications:

1. Mehra, P.; **Paul. A.*** Covalently Functionalized Hydroxyl-rich Few-layer Graphene for Solid-state Proton Conduction and Supercapacitor Applications. *J. Phys. Chem. C* **2022,** *126*, 6135-6146.
2. Sharma, S.; Roy, A.; Shaw, K.; Bisai, A.*; **Paul, A.*** Electrochemical Synthesis of Dimeric 2-Oxindole Sharing Vicinal Quaternary Centers Employing Proton-Coupled Electron Transfer (PCET). *J. Org. Chem.* **2020**, *85*, 14926-14936.
3. Jash, P.; **Paul, A.*** Selective synthesis of single layer translucent cobalt hydroxide for the efficient oxygen evolution reaction. *Chem. Commun.* **2019**, *55*, 2230-2233.
4. Saha, J.; Roy Chowdhury, D.; Jash, P.; **Paul, A.*** Cobalt phosphonates as precatalysts for water oxidation: Role of pore size in catalysis. *Chem. Eur. J.* **2017**, *23*, 12519-12526.
5. Singh, C.; S. N.; Jana, A.; Mishra, A. K.*; **Paul, A.*** Proton conduction through oxygen functionalized few-layer graphene. *Chem. Commun.* **2016**, *52*, 12661-12664.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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Functional group-based approach to the heterocycle synthesis

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Abstract:
Metal catalyzed transformations of alkynes have gained prominence for the synthesis of *oxa*- and *aza*-cycles. However, their utility under metal free conditions is still under explored. In this context, we have demonstrated that the oxonium and iminium ion intermediates generated from vinylogous carbonates and carbamates in the presence of Lewis acids can be trapped with alkynes to get access to 2,3-disubstituted dihydrobenzofurans and indoline derivatives. Over the years, these studies were extended to divergent synthesis of heterocycles such as indoles, quinolines, cyclic ethers and amines and cyclic acetals under not only Lewis acidic conditions but also under radical conditions (Figure 1). The talk will focus on some of the recent developments on using alkynes for the synthesis of heterocycles from our laboratory.

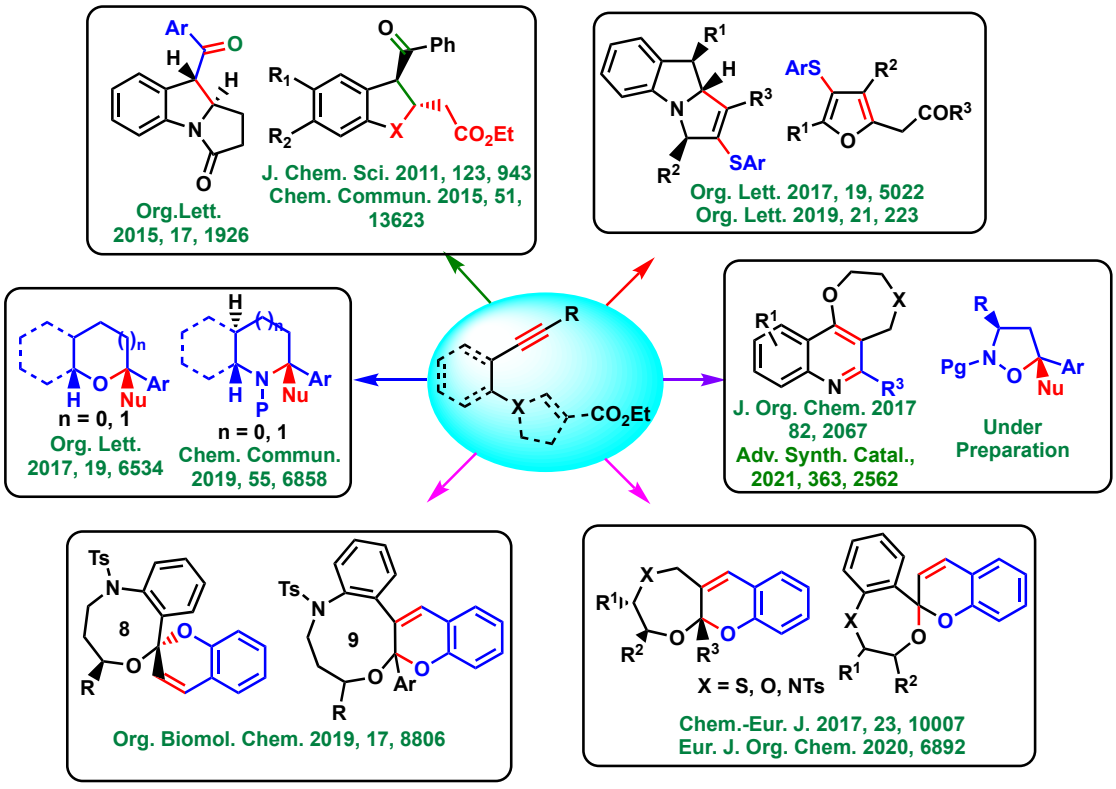

Fig. 1: Alkynes in the synthesis of heterocycles

References and Notes:

1. Gharpure, S. J.; Nanda, S. K.; Fartade, D. J. *Adv. Synth. Catal.*, **2021**, *363*, 2562.
2. Gharpure, S. J.; Nanda, S. K.; Fartade, D. J. *Org. Biomol. Chem.*, **2019**, *17*, *8806.*
3. Gharpure, S. J.; Vishwakarma, D. S.; Patel, R. K. *Chem. Commun.*, **2019**, *55*, 6858.
4. Gharpure, S. J.; Padmaja; Prasath, V.; Shelke, Y. G. *Org. Lett.*, **2019**, *21*, 223.

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Dr. Santosh J. Gharpure graduated with an M.Sc. degree in 1996, from Indian Institute of Technology Bombay, Powai. He obtained Ph.D. from Indian Institute of Science, Bangalore working with Late Prof. A. Srikrishna in 2001. He held a post-doctoral position with Prof. P. Andrew Evans at Indiana University, Bloomington, U.S.A. Subsequently, he joined the Department of Chemistry, IIT Madras, Chennai in the year 2004. In 2012, he moved to the Department of Chemistry, IIT Bombay, Powai, Mumbai as an Associate Professor and was promoted to Professor position in 2016. Currently, he holds the position of 'Rasiklal Hemani Fragrance and Flavour Chair Professor'. He is also Professor In-Charge of SINE, IIT Bombay's technology incubator. His research focuses on organic chemistry pertaining to natural and unnatural product synthesis and developing new synthetic methodologies. He is also working on problems relevant to industries from different domains.

Dr. Gharpure is a recipient of INSA Medal for Young Scientist. He was awarded IIT Madras Young Faculty Recognition Award (YFRA) for his contribution in teaching and research in 2010. He received B. M. Birla science Prize in Chemistry for the year 2011. He was selected as one of the Thieme Chemistry Journal Awardees for the year 2013. IIT Bombay conferred on him the Excellence in Teaching Award in the year 2015 and Departmental award for excellence in teaching in 2019. He was selected as Themis Medicare UICT Diamond Jubilee Distinguished Fellow in Pharmaceutical Science for the year 2015-16 of ICT, Mumbai. He was selected for the award of Chemical Research Society of India (CRSI) Bronze Medal in 2018. He is member of the International Advisory Board of European Journal of Organic Chemistry. He is a Fellow of Royal Society of Chemistry (FRSC). Very recently, he was awarded INSA Teachers Award 2021 by Indian National Science Academy, New Delhi.

Crystallization-Driven Controlled Two-Dimensional (2D) Assemblies from Chromophore-Appended Poly(L-lactide) Homopolymers

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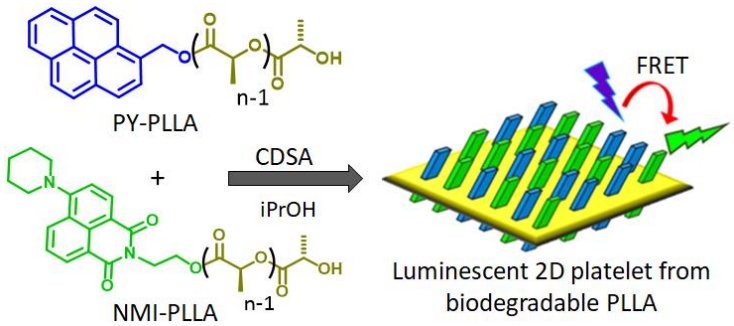
Abstract:
Supramolecular assemblies of functional π-conjugated systems are majorly restricted to spherical or one-dimensional (1D) structures with limited examples reported on their two-dimensional (2D) architectures. Crystallization-driven self-assembly (CDSA) of semicrystalline block copolymers (BCPs) has recently emerged as a powerful technique for fabrication of diverse hierarchical anisotropic structures, including 2D architectures. In this present work, we showcase a new development made in the field of CDSA of chromophore-conjugated poly(L-lactide)s (PLLAs) for programmed synthesis of discrete 2D architectures with exciting photophysical properties and predictable morphologies. PLLA homopolymers, end-functionalized with different dipolar chromophores such as merocyanine (MC) or naphthalene monoimide (NMI) and nonpolar pyrene (PY) or benzene (Bn) crystallize into precise diamond-shaped 2D platelets in isopropanol under suitable condition. This causes the terminally attached chromophores to assemble into 2D array on the platelet surface by either dipole-dipole interactions (for NMI and MC) or aromatic stacking (PY and Bn), which leads to the aggregation-induced enhanced emission (AIEE) with tunable emission wavelengths within the 2D crystals, depending upon the nature of the end-capped chromophores. Further, co-assembly between NMI- and PY-functionalized PLLAs yielded similar two-component co-platelets with highly efficient Förster Resonance Energy Transfer (FRET) from the donor (PY) to the acceptor (NMI) dye with remarkable efficiency (~80%) on the 2D surface. Moreover, "living" CDSA method was employed to achieve hierarchical segmented block co-platelet structures using one of the homopolymer platelets as the "seed", and the unimer of the other as the "monomer reservoir".



References and Notes:

1. Rajak, A.; Das, A. *Angew. Chem. Int. Ed.* **2022**, *61*, e202116572. (Selected as a Hot Paper and Cover Picture)

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

Anindita Das
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Anindita Das received her Ph.D. from the Indian Association for the Cultivation of Science (IACS), Kolkata, India in 2014 under the supervision of Professor Suhrit Ghosh. Subsequently, she worked as an Alexander von Humboldt Postdoctoral Fellow with Professor Patrick Théato at the University of Hamburg, Germany during 2014-2016. In 2016, she joined the group of Professor E. W. Meijer at the Eindhoven University of Technology, The Netherlands, for a second postdoctoral stint. In 2017, she joined at IACS as a Faculty Fellow, where she currently holds the position of Assistant Professor in the School of Applied and Interdisciplinary Sciences. Her research interests include supramolecular assemblies of functional π-systems and macromolecules employing halogen bonding and other underexplored supramolecular interactions, crystallization-driven macromolecular assemblies and biodegradable polymers.

Selected Publications:

1. A. Rajak, **A. Das*** "Crystallization-Driven Controlled Two-Dimensional (2D) Assemblies from Chromophore-Appended Poly(L-lactide)s: Highly Efficient Energy Transfer on a 2D Surface", *Angew. Chem. Int. Ed.* **2022**, *61*, e202116572. (Selected as a Hot Paper and Cover Picture)
2. A. Jamadar, A. K. Singh, L. Roy,* **A. Das**,* "Stimuli-Responsive Luminescent Supramolecular Assemblies and Co-assemblies by Orthogonal Dipole-Dipole Interaction and Halogen Bonding", *J. Mater. Chem. C* **2021**, *9*, 11893. (Featured in the Emerging Investigators' special issue 2021)
3. A. Jamadar,ǂ C. K. Karan,ǂ S. Biswas,ǂ **A. Das*** "Structural Influence on Stimuli-Responsive Halogen-Bonded Luminescent Supramolecular Polymers from Heteroditopic Isomers", *CrystEngComm* **2021**, *23*, 1695. (ǂ equal contribution) (Featured as Cover Picture)
4. A. Rajak, C. K. Karan, P. Théato, **A. Das**,* "Supramolecularly Cross-linked Amphiphilic Block Copolymer Assembly by Dipolar Interaction of a Merocyanine Dye", *Polym. Chem*. **2020**, *11*, 695. (Featured as Cover Picture)
5. A. Jamadar, **A. Das**,* "pH-Responsive Graftable Supramolecular Polymer with Tailorable Surface Functionality by Orthogonal Halogen Bonding and Hydrogen Bonding", *Polym. Chem*. **2020**, *11*, 385. (Featured in the Emerging Investigators' special issue 2020)

Awards/Achievements:

- DAE-BRNS Young Scientist Research Award 2022.
- Author's Profile Published in *Angew. Chem. Int. Ed.* 2022.
- Early Career Advisory Board Member of the Journal *ChemNanoMat* since 2022.
- Editorial Board Member of the *Journal of Macromolecular Science, Part A: Pure and Applied Chemistry* since 2022.
- IUPAC-Solvay International Award for Young Chemists (2015) for best PhD thesis under Honorable Mention Award Category.
- Alexander von Humboldt Postdoctoral Fellowship 2014.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
…Anticipating Tomorrow's Science through Collaborative Ventures

Dr. Sandip Murarka

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Sandip Murarka did his B.Sc. in Chemistry (Hons.) from Midnapore College, Vidyasagar University (2005), and M.Sc. from IIT Bombay (2007). Subsequent to a M.S. from Rutgers University, U.S.A (2009); he moved to Germany to pursue his PhD from WWU Münster under the supervision of Prof. Armido Studer. After completion of his Ph.D. (2013), he worked as a Max-Planck postdoctoral research fellow in the laboratory of Prof. Herbert Waldmann at Max Planck Institute of Molecular Physiology, Dortmund (2013-2016). Following a year long stay (2016-2017) as a Team Leader in a reputed pharmaceutical company, Syngene International Limited, he decided to move back to academia. In May 2017, he joined Indian Institute of Technology Jodhpur, India as an Assistant Professor and got promoted to the post of Associate Professor in June 2022. His current research activities include study of novel activation modes and development of chemoselective and sustainable transformations towards the synthesis of biologically relevant and interesting molecular architectures.

Awards:

1. 'Thieme Chemistry Journal Award' by the editorial boards of the journals Synthesis, Synlett, and Synfact (2022).
2. Early Career Advisory Board Member of Wiley-VCH Journal 'ChemistrySelect' (2022).
3. Fellow of Indian Chemical Society (2020).
4. Early Career Research Award (ECRA) from Science and Engineering Research Board (SERB) (2018).
5. INSPIRE Faculty Award from the Department of Science & Technology (DST), India (2016).

Representative Publications:

1. Multicomponent Synthesis of Biologically Relevant *S*-Diarylmethane Dithiocarbamates Using *p*-Quinone Methides, S. K. Parida, S. K. Hota, S. Jaiswal, P. Singh, S. Murarka, *Adv. Synth. Catal.* **2022**, 364, 1549. *Selected as a Very Important Publication (VIP)*.
2. Multicomponent synthesis of biologically relevant *S*-aryl dithiocarbamates using diaryliodonium salts, S. K. Parida, S. Jaiswal, P. Singh, S. Murarka, *Org. Lett.* **2021**, 23, 6401.
3. Single Electron Transfer-Induced Redox Processes Involving *N*-(Acyloxy)phthalimides, S. K. Parida, T. Mandal, S. Das, S. K. Hota, S. De Sarkar, S. Murarka, *ACS Catal.* **2021**, *11*, 1640.
4. *N*-(acyloxy)phthalimides as Redox-Active Esters in Cross Coupling Reactions, S. Murarka, *Adv. Synth. Catal.* **2018**, *360*, 1735. Selected as a *Very Important Publication (VIP)*. Top 10% most downloaded paper.

Role of Chemistry in Developing Durable & Different Bio-inspired Liquid Wettability

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Abstract:

The nature-inspired wettabilities that either extremely repelled or allowed effortless sliding of different liquids (oil/water) in air or underwater are with immense potential for various prospective applications. In common practice, essential chemistry and appropriate topography that conferred the special liquid wettabilities were mostly and generally achieved by associating delicate chemistry. Eventually, the synthesized materials suffered from poor durability issue. In the literature, very few designs are capable of providing durable bio-inspired wettability—but fabrication processes remained generally complex. Moreover, the integration of various other relevant physical properties with such durable liquid wettability is highly challenging to achieve. Hence, design of robust bio-inspired liquid wettability following simple fabrication process that would allow to integrate different and relevant physical property is utmost important for various fundamental and applied contexts. Related to this, recently, our research group have extended 1,4 conjugate addition reaction between amine and acrylates at ambient condition to develop tolerant and functional liquid wettability.[1-5] The controlled tailoring of different bio-inspired liquid wettability from the porous and chemically reactive interfaces—following strategic post modulation of the chemically reactive interfaces will be discussed in this invited lecture. Even, a strategic association of adequate crosslinkers can provide a highly tolerant and hard superhydrophobic coating on a geometrically complex and soft materials. Such simple chemical approach also allowed to reveal important fundamental aspects related to different bio-inspired wettability. Taking advantage of the durable bio-inspired wettability, the synthesized nature inspired interfaces were successfully applied to demonstrate some practically relevant applications—including controlled release of small molecules, oil/water separation, water harvesting, strain sensing, controlled bubble transport etc.[1-5]

References and Notes:

1. Shome, A.; Das, A. Borbora, A.; Dhar, M.; Manna, U. *Chemical Society Reviews*, **2022,** In Press.
2. Dhar, M.; Das, A.; Parbat, D.; Manna, U. Angewandte Chemie International Edition, **2022**, 61, e20211676.
3. Borbora, A.; Dupont, L. R.; Xu, Y.; Wang, X.; Manna, U. *Materials Horizon,* **2022**, 9, 991-1001.
4. Shome, A.; Das, A.; Manna, U.; *Chem. Mater.*, **2021**, 33, 8941–8959.
5. Baruah, U.; Manna, U. *Chem. Sci.*, **2021**, 12, 2097–2107.

Bio-Sketch of Speaker

Name: Uttam Manna, FRSC
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Dr. Uttam Manna, an Invited Fellow of the Royal Society of Chemistry (FRSC), currently an associate professor at the Indian Institute of Technology Guwahati, completed his PhD at IISc Bangalore in 2011. He pursued his postdoctoral research at the University of Wisconsin–Madison from 2011 to 2015. He has been selected as an associate of the Indian Academy of Sciences in 2018. He is a recipient of both the NASI-Young Scientist Platinum Jubilee Award-2018 and INSA-Medal for Young Scientist-2019. *Journal of Materials Chemistry A* (2018), *Chemical Communications* (2020) and Nanoscale (2021) recognized him as an emerging investigator. Currently, he is in the advisory board member of *Materials Horizons, RSC and ACS Applied Engineering Materials, ACS*. His research team is involved in designing functional and durable bio-inspired wettability through strategic use of catalyst free and simple chemical reactions at ambient condition.

Title: Glucose-responsive hydrogels towards artificial pancreas

Author(s) name:Suchetan Pal*, Akbar Ali
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Abstract: According to the world health organization (WHO), diabetes is one of the leading causes of death and poses a global epidemic in the coming decades. All type 1 and advanced stage type 2 diabetes patients rely on administration of insulin, a peptide hormone normally secreted in pancreas and responsible for blood glucose metabolism. Daily inconvenient and painful subcutaneous injection remains the primary route of insulin delivery in such patients. Another major drawback of traditional insulin delivery is the increased risk of potentially fatal hypoglycemia due to the premature action. Therefore, major research studies are being carried out to alleviate these issues. Micro and nanotechnology-based insulin carriers are undergoing major development for non-invasive and/glucose responsive delivery of insulin. In this abstract, we elaborate about our recent results on glucose-responsive delivery of insulin for biocompatible hydrogels. We fabricate hydrogels by crosslinking biocompatible polymers and biomolecules such as proteins using bifunctional crosslinkers that create extended three-dimensional networks. I will present three different generations of polymer- protein hybrid gels developed in our laboratory that show excellent insulin release properties in physiological conditions. In future, such biomematic insulin delivery systems will be explored for low cost long-acting insulin and potential artificial pancreas.

Figure/Scheme (if any):

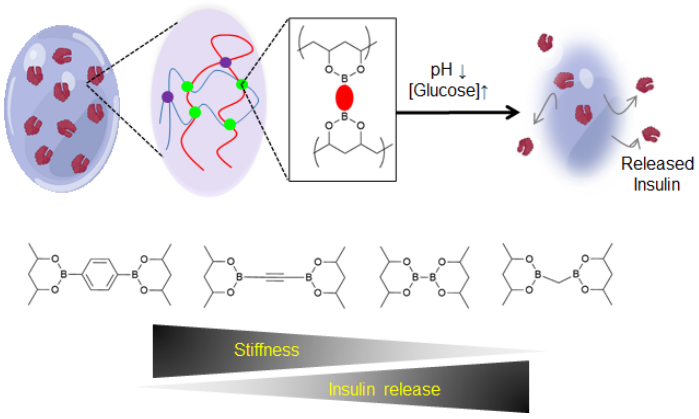

Figure 1: Glucose responsive hydrogels show glucose concentration dependent degradation and insulin release under hyperglycaemic conditions.

References and Notes:

1. Ali, A.; Nauseen, S.; Saroj, S.; Shegane, M.; Majumder, P.; Puri, A.; Rakshit, T.; Manna, D.; Pal, S. Journal of Materials Chemistry B, 2022 (accepted)
2. Ali, A.; Nagumantri, S. P.; Rakshit, T.; Pal, S. Macromolecular Chemistry and Physics 2021, 222, 2100121.

Bio-Sketch of Speaker

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Dr. Suchetan Pal obtained his B. Sc. and M. Sc. in Chemistry from Jadavpur University and Indian Institute of Technology, Kanpur respectively. Then, he joined Arizona State University, for his doctoral studies. After completing the thesis work on "DNA directed self-assembly of plasmonic nanoparticles," Dr. Pal moved to a joint post-doctoral position at Columbia University and Brookhaven National Laboratory. He had completed another postdoctoral stint at the Memorial Sloan Kettering Cancer Center, before joining Indian Institute of Technology, Bhilai as an assistant professor. His primary research focus includes biomolecular nanotechnology for drug delivery, biosensing and bioimaging.

Awards:

- Young Investigator Award 2021 from the Society of Interdisciplinary Research in Materials and Biology (SIRMB).
- Hargovind Khorana Young Innovative Biotechnologist Award-2019 by DBT, GOI.
- INSPIRE Faculty award by DST, GOI July 2016 (not availed).
- Eyring memorial award for best research scholar in the year 2011 by Department of Chemistry and Biochemistry, Arizona State University.

Representative Publications:

- **Journal of Materials Chemistry B.** 2022.
- **Macromolecular Chemistry and Physics.** 2021.
- **Nature Communications.** 2019.
- **Advanced Functional Materials.** 2017.

Janardan Kundu

Designation: Assistant Professor

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Janardan received his Doctoral degree from Rice University, Houston, TX- USA in 2010 and was a post-doctoral research scholar at Los Alamos National Lab, Los Alamos, New Mexico, USA during 2010-2013. He joined CSIR-NCL Pune as a Ramanujan fellow in the Physical and Materials Chemistry division (2014-2018) and moved to Indian Institute of Science Education and Research Tirupati to join as Assistant Professor in Chemistry Department in 2018. His primary research interest is on experimental material chemistry involving multifunctional materials (metal, semiconductor, heterostructures) for Energy and Environment. Currently, his group focusses on low dimensional metal halide hybrids for broad-band emission. Structure-property relationship in such material is currently being pursued by his group at Tirupati.

Selected Publications:

1) Synergistic Electronic Coupling/Cross-talk between the Isolated Metal Halide Units of Zero Dimensional Heterometallic (Sb, Mn) Halide Hybrid with Enhanced Emission. J. Mater. Chem. C 2022, 10, 360-370;

2) Lead-Free Zero-Dimensional Tellurium (IV) Chloride-Organic Hybrid with Strong Room Temperature Emission as Luminescent Material. J. Mater. Chem. C 2021, 9, 4351-4358; DOI: 10.1039/D0TC05752E;

3) The Metal Halide Structure and the Extent of Distortion Control the Photo-Physical Properties of Luminescent Zero Dimensional Organic-Antimony(III) Halide Hybrids. J. Mater. Chem. C 2021, 9 (1), 348–358; DOI: 10.1039/d0tc03440a;

4) Efficient Broad-Band Emission from Contorted Purely Corner-Shared One Dimensional (1D) Organic Lead Halide Perovskite. Chem. Mater. 2019, 31 (7), 2253–2257; DOI: 10.1021/acs.chemmater.9b00069;

5) Efficient Exciton to Dopant Energy Transfer in Mn2+-Doped (C4H9NH3)2PbBr4 Two-Dimensional (2D) Layered Perovskites. Chem. Mater. 2017, 29 (18), 7816–7825; DOI: 10.1021/acs.chemmater.7b02429;

Near-IR, Not Too Far: Handcuffing the Bays of Terrylene Diimide

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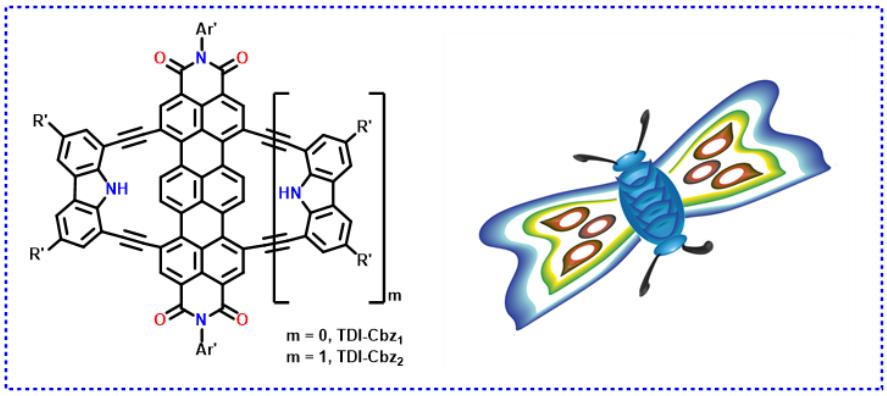
Abstract:
Molecules emitting in Near-infrared (NIR) region are in demand for their utility in night vision detectors and biological imaging. Even though a handful of NIR absorbing molecular classes are known, reports on intense NIR emitting molecules are sparse. Longer rylene diimides such as terrylene diimides (TDIs) are important class of molecules having intense absorption and emission in the NIR range.[2] However, these larger polyaromatics hinder their synthesis, isolation and characterization due to inherent aggregation. Herein, we present an interesting way to achieve novel Janus butterfly-shaped TDI-carbazole derivatives. These new molecules have intense absorption and emission in the range of 720 nm – 897 nm. The emission quantum yields observed are some of the highest among this class of molecules (up to **93%**).[3] We also present the serendipitously obtained two-tiered TDI derivative **(TDI-Cbz$_4$)** having an emission maxima at 897 nm. This work highlights the utility of precise electronic and structural tuning necessary to achieve intense NIR absorbing and emitting molecules for modern applications.



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1. Law, K.Y.; *Chem. Rev.*, **1993**, *93*, 449-486.
2. Holtrup, F. O.; Müller, G. R. J.; Quante, H.; Feyter, S. De.; Schryver, F. C. De.; Müllen, K.; *Chem. Eur. J.*, **1997**, *3*, 219-225.
3. Mehra, K. S.; Jha, S.; Bhandary, S.; Mandal, D.; Mishra, R.; Sankar, J.; *Angew. Chem. Int. Ed.*, **2022,** *https://doi.org/10.1002/anie.202205600*

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

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After completing his PhD from IIT Kanpur (2005) and JSPS Fellowship (2008) from Kyoto University, he joined IISER Bhopal as an assistant professor in 2009. Currently, he is at the same institute as a full professor. His group is interested in developing new molecules with polyaromatic backbone for modern molecular electronic applications. Metal complexes of bio-inspired macrocycles too are being investigated with the aim to utilize them as magnetic materials and redox-active catalysts.

Selected Publications:

1. Bridging the Bays, Both Ways: A Janus Butterfly-shaped Intense NIR-Emitting Terrylene Diimide
   Mehra, K. S; Jha, S; Bhandary, S; Mandal, D; Sankar, J.
   Angew. Chem. Int. Ed. **2022**, e202205600.
2. Isolation and Structural Characterization of Regioisomers of Dibrominated Terrylene Diimides
   Jha, S; Mehra, K. S.; Hasija, A; Chopra, D; Regar, R; Sankar, J.
   J. Org. Chem. **2022**, *87*, 5, 3770–3774.
3. A NIR Absorbing Ortho-pi-extended Perylene Bisimide as Promising Material for Bulk Heterojunction Organic Solar Cell
   Regar, R; Mishra, R; Singhal, R; Sharma, G. D.; Sankar, J.
   J. Mater. Chem. A, **2019**, *7*, 3012–3017
4. The Curious Case of a Parasitic Twin of the Corroles
   Basumatary, B; Reddy, R. V. R; Rahul; Sankar, J.
   Angew. Chem. Int. Ed., **2018**, *57*, 5052-5056

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Intermolecular Dearomative [4+2] Cycloaddition of Naphthalenes via Visible-Light Energy-Transfer-Catalysis

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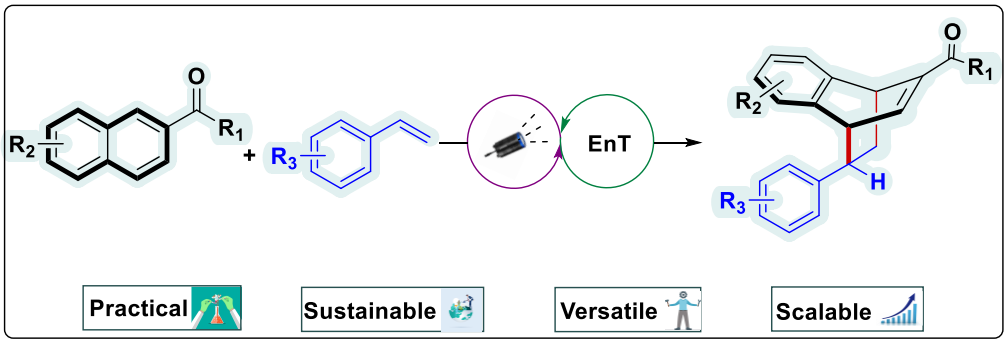
Abstract:
Dearomative cycloaddition reaction serves as a blueprint for creating three-dimensional molecular topology from flat-aromatic compounds.[1,2] However, dearomative cycloaddition of arenes system is highly challenging because of the high chemical stability inherent due to aromaticity. Further, severe reactivity, selectivity and reversibility issues make this process arduous.[1,2] One such process to overcome these challenges is the photochemical approach that induces the loss of aromaticity.[1,2] Visible-light photocatalysis, in particular, has developed as an effective and ecologically beneficial mechanism for exploiting energy transfer and electron transfer, allowing for sustainable reactions including diverse dearomative reactions. Chemists have developed a number of dearomative transformations of arenes via visible light catalysis, which are now essential tools for the synthesis of complex molecular scaffolds. In this regard, the current presentation emphasises the difficult issues of the dearomative cycloaddition reaction.[3] Firstly, a brief overview of the current state of the art of dearomative cycloaddition reaction will be discussed. The introduction will be followed by a discussion of possible reaction conditions to mitigate the problems. The presentation will focus on how the visible light energy transfer process can be accessed for the cycloaddition reaction of feed-stock naphthalene molecules with vinyl benzenes where, structurally diverse 2-acyl naphthalenes, and styrenes with various functional groups could easily be converted to a diverse range of bicyclo[2.2.2]octa-2,5-diene scaffolds in high yields and selectivities. The presentation will shed light on visible light energy transfer catalysis which is in the early stage of the chemical synthesis.

Figure/Scheme:



References and Notes:

1. Remy R., Bochet C. G., *Chem. Rev.* **2016**, *116*, 9816-9849
2. Ma J., Chen S., Bellotti P., Guo R., Schäfer F., Heusler A., Zhang X., Daniliuc C., Brown M. K., Houk K. N., Glorius F., *Science* **2021**, *371*, 1338-1345
3. Rai P.; Maji K.; Jana S. K.; Maji B*, 2022, 10.26434/chemrxiv-2022-93cks

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1987: Born, Howrah, India
2007: B.Sc. University of Calcutta (Chemistry Hons.)
2009: M.Sc. Indian Institute of Technology Kanpur (Chemistry)
2012: PhD Ludwig Maximillan Universität Munich, Supervisor: Prof. Herbert Mayr
2013-2015: Postdoc: Chubu University, Mentor: Prof. Hisashi Yamamoto
2016: Alexander von Humboldt fellow: Westfälische Wilhelms-Universität Münster, Mentor: Prof. Frank Glorius
2016-2021: Assistant Professor, Indian Institute of Science Education and Research Kolkata
2021-: Associate Professor, Indian Institute of Science Education and Research Kolkata

Research focus: Organic synthesis, catalysis, and mechanistic studies.

Awards:
2021: "2021 Young Investigator Award ", Sponsored by Molecules
2021: Merck Young Scientist Award (runner-up) in Chemical Science
2021: INSA Medal for Young Scientists
2021: Associate of the Indian Academy of Sciences (IASc)
2020: NASI-Young Scientist Platinum Jubilee Award (2020) in Chemical Sciences
2019: Thieme Journal Award

Selected publication:

- K. Das, S. Waiba, A. Jana, B. Maji, *Chem. Soc. Rev.* **2022**, *51*, 4386-4464.
- A. Jati, K. Dey, M. Nurhuda, M. A. Addicoat, R. Banerjee, B. Maji, J. *Am. Chem. Soc.* **2022**, *144*, 7822-7833.
- S. Waiba, M. Maiti, B. Maji, *ACS Catalysis* **2022**, *12*, 3995-4001.
- S. K. Jana, M. Maiti, P. Dey, B. Maji, *Org. Lett.* **2022**, *24*, 1298-1302.
- K. Das, K. Sarkar, B. Maji, *ACS. Catal.* **2021**, *11*, 7060-7069.
- K. Sarkar, K. Das, A. Kundu, D. Adhikari, B. Maji, *ACS. Catal.* **2021**, *11*, 2786-2794.
- A. Jana, K. Das, A. Kundu, P. R. Thorve, D. Adhikari, B. Maji, *ACS Catal.* **2020**, *10*, 2615-2626.

Bio-Sketch of Speaker

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Dr. Mandal joined the Department of Chemistry, IIT Ropar in 2010. His research work is centred around Inorganic and Organometallic Chemistry and this core area branches into catalysis, organic synthesis, and recoverable catalysts, particularly those with fluorous "ponytails" of the formula $(CH_2)_m(CF_2)_nF$. Recently his group started working on Li-ion, Li-sulphur battery, Ionic Liquids, Ionic Polymers, Composites of Polyoxometallate as electrocatalyst and sensors. Dr. Mandal worked with Prof. Gladysz group at Erlangen, Germany as an Alexander von Humboldt Foundation (AvH) fellow for post-doctoral study after his PhD at IIT Kanpur. Then he moved to Texas A&M University where he was working mainly on methane oxidation (industrial project) for more than two years before joining IIT Ropar.

Education:
Ph.D., Indian
Institute of Technology Kanpur, 2006

M.Sc., Banaras Hindu University, 2000

B.Sc., Midnapore College (Vidyasagar University), 1998

Deciphering Importance of Molecular Interactions and Hydration Dynamics in Physical Biology

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Abstract:

The molecular interactions and dynamics of hydration are key for functioning of biological macromolecules. In fact, water around biomolecules is special for behaving strangely both in terms of its structure and dynamics, while both water and ions are found to control various molecular interactions of nucleic acids, proteins and lipids. Understanding such fundamental processes is at the core of physical biology. The questions, how water and ions around biomolecules behave dynamically and how they affect the molecular interactions involving such biomolecules, have triggered tremendous research activities worldwide. Such activities not only unfolded important static and dynamic properties of water and ions around biomolecules and their roles in bimolecular functions, but also provoked heated debate for decades. This talk will showcase a board overview of the research from our laboratory, together with other labs, which encompasses understanding the fundamental basis of physical biology using fluorescence experiments and computer simulation, particularly on DNA and lipid membrane, which unfolded several interesting dynamic features of these biomolecule. Most importantly, the talk will showcase how direct comparison of experimental and computer simulation results can unfold the ultimate molecular details of such interactions and dynamics of biomolecules.

Bio-Sketch of Speaker

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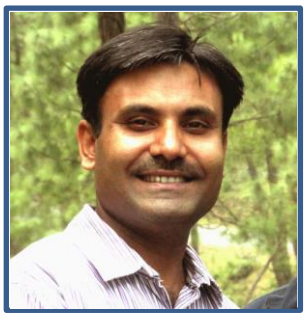

Career Profile

Associate Professor, School of Physical Sciences, Jawaharlal Nehru University, New Delhi (2014 - present).
Assistant Professor, School of Physical Sciences, Jawaharlal Nehru University, New Delhi (2007 - 2014).
JSPS Postdoctoral Fellow at Molecular Spectroscopy Laboratory, RIKEN, Wako, Saitama, Japan (2005 - 2007).
Postdoctoral Fellow at the Department of Chemistry and Biochemistry, University of South Carolina, USA (2003 - 2005).

Awards/Achievements

2022 - Editorial Board Member of *Journal of Chemical Sciences*
2020 - Editorial Board Member of *Chemical Physics Impact*
2017 - Invited Institute Seminar at S. N. Bose National Centre for Basic Sciences, Kolkata
2015 - Invited (Wednesday) Colloquium at Tata Institute of Fundamental Research, Mumbai
2012 - Asian and Oceanian Photochemistry Association (APA) Young Scientist-2012 Award
2005 - Japanese Society for the Promotion of Science (JSPS) Fellowship

Representative Publications

1. Yadav et al. *J. Phys. Chem. B* **2022**, *126*, 1668.
2. Sardana et al. *J. Phys. Chem. B* **2019**, *123*, 10202.
3. Singh et al. *Phys. Chem. Chem. Phys.* **2016,** *18*, 24185.
4. Pal et al. *J. Phys. Chem. Lett.* **2015**, 6, 1754.
5. Verma et al. *Anal. Chem.* **2012**, 84, 7218.
6. Sharma et al. *J. Am. Chem. Soc.* **2012**, 134, 19677.
7. Verma et al. *J. Phys. Chem. Lett.* **2012**, 3, 2621.
8. Pal et al. *Anal. Chem.* **2011**, 83, 7736.
9. Pal et al. *J. Am. Chem. Soc.* **2010**, 132, 9277.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

S-aryl dithiocarbamate: Novel small molecule inhibitors involved in tubulin bundling

Author(s) name: Sonal Jaiswal[1]‡, Sushanta K. Parida[2]‡, Sandip Murarka[2]* and **Priyanka Singh[1]***

[1]*Department of Bioscience & Bioengineering, Indian Institute of Technology Jodhpur, India*
[2]*Department of Chemistry, Indian Institute of Technology Jodhpur, India*

(Email: priyankasingh@iitj.ac.in; sandipmurarka@iitj.ac.in)

Abstract:

Cancer is a leading cause of global human deaths. It is characterized by uncontrolled cell division which causes genomic instability. Identification of new chemical entities with novel structure and biological functions is imperative to the advancement of cancer chemotherapeutics. Dithocarbamates belongs to a versatile class of organosulfur compounds with anti-bacterial, antifungal and anti-inflammatory roles. There are only a few reports about their anti-inhibitory effects in cancer cells, which mostly uses S-*primary* alkyl dithiocarbamates. We recently identified that *S*-secondary alkyl also have good inhibitory activity in cancer cell lines.[1] Next, we found using *in silico* analysis that the *S*-aryl dithiocarbamates synthesized by utilizing transition metal-free one-pot multicomponent method exhibit good drug-likeness and pharmacophore properties.[2] We could validate that the lead compound from *in silico* analysis had antiproliferative activity in cancer cell lines with low micromolar IC_{50} value. Further investigation revealed that the lead compound induce G_2/M cell cycle arrest and increase in cell apoptosis *via* the p53-p21 signaling pathway. Interestingly, we observed microtubule bundling in cells treated with our lead compound, which is a characteristic phenotype of microtubule-stabilizing drugs like paclitaxel. Thus, our work lead towards identification of a S-aryl dithiocarbamate moiety as a promising novel candidate for drug discovery in cancer chemotherapeutics.

Figure/Scheme (if any):

References and Notes:

1. Parida, S. K.[+].; Hota, S.K.[+]; Jaiswal, S. J.; Singh, P.*; Murarka, S.* *Advanced Synthesis & Catalysis* **2022**, 364, 1549-1554. Selected as a Very Important Publication (VIP).
2. Parida, S. K.; Jaiswal, S. J.; Singh, P.*; Murarka, S.* *Organic Letters* **2021**, *23*, 6401-6406.

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

Name: Priyanka Singh

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Recent Picture

Career Profile, significant awards/achievements and representative publications

Dr. Priyanka Singh has worked in diverse fields of life sciences and gained interdisciplinary skill sets. Her doctoral work provides understanding of possible interplay between the tumor suppressor proteins and proto-oncogenes which upon misregulation results in various human cancers (*Nucleic Acids Research 2015*, *Oncogene 2014*, *Journal of Biological Chemistry 2011*, *Oncogene 2011*, *Oncogene 2009*). As an *EMBO-Long Term Fellow*, she investigated molecular link between asymmetric behavior of the major microtubule organizing centers *i.e.*, centrosomes and timely spindle formation, which decides the division axis in asymmetrically dividing *Drosophila* neural stem cells (*Cell Reports 2016*, *Current Biology 2014*). As *Humboldt (AvH) fellow*, she was involved in identifying the relationship between molecular players present at kinetochores (multi-subunit complexes built on centromeric chromatin) and spindle assembly checkpoint during the cell division (*Molecular Cell 2021*, *eLife 2016*, *eLife 2017*).

Presently, Dr. Priyanka Singh is working as an Assistant Professor at IIT Jodhpur. She is the recipient of several prestigious and competitive national level awards which include *Young Scientist Research Award-2021* (BRNS), *Innovative Young Biotechnologist Award-2019* (DBT) and *Early Career Research Award-2018* (SERB). Her research group at IITJ is utilizing interdisciplinary skillsets to investigate mechanisms of centrosome organization and cell proliferation (*Methods in Cell Biology 2021*, *Seminars in Cell & Developmental Biology 2021*, *Journal of the Indian Institute of Science 2021*, *Cells 2018*). As a collaborative effort, her lab is utilizing forward and reverse drug discovery approach, in order to identify novel anti-cancerous molecules (*Advanced Synthesis & Catalysis 2022*, *Organic Letters 2021*). In nutshell, she is taking a holistic approach to establish prognostic and diagnostic value of

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
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Rajarshi Samanta

Recent Picture

Associate Professor

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B. Sc. & M. Sc.:
B.Sc.: Jadavpur University, Kolkata, India, 2002
M.Sc.: Jadavpur University, Kolkata, India, 2004 (Mentor: Professor Rina Ghosh)

Ph.D.: Indian Institute of Chemical Technology, Hyderabad, 2010.
(Mentor: Professor Tushar Kanti Chakraborty)

Postdoctoral Tenure:
- Max Planck Institute of Molecular Physiology, Dortmund. June 2010-Sep 2013. (Mentor: Dr. Andrey P. Antonchick)

Employment:

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

Fellowships/Honours:
- Associateship for the Indian Academy of Sciences (2019-2022)
- Emerging Investigator: New J Chem, 2021
- Max-Planck Fellowship
- CSIR JRF/SRF, GATE (AIR 11)
- National Scholarship

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

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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Catalytic Functionalization of Metallocarbenes Derived from α-Diazocarbonyl Compounds and Its Surrogates

Pazhamalai Anbarasan
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Indian Institute of Technology Madras, Chennai-600036
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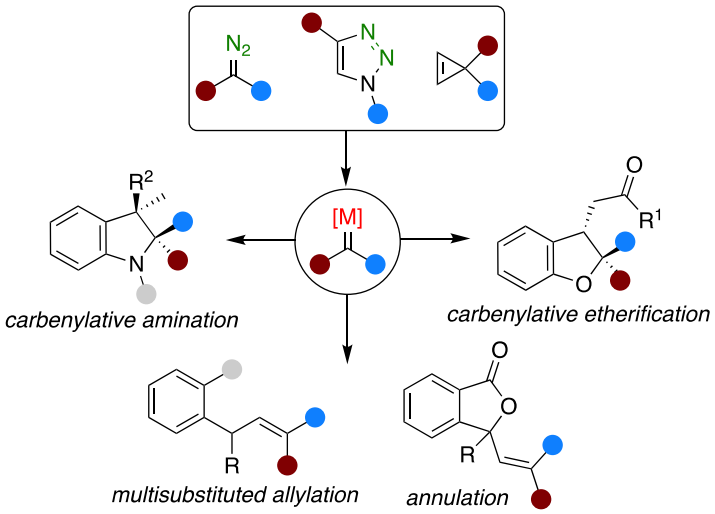
Abstract:
Metallocarbenes show versatile reactivity in organic synthesis and offers access to diverse complex frameworks in single step. Most often these metallocarbenes are generated from α-diazocarbonyl compounds in the presence of suitable transition metal.[1] Recently, *N*-sulfonyl-1,2,3-triazoles and cyclopropenes have emerged as unique surrogates and offers structurally different metallocarbenes, which possess distinct reactivity.[2] The unique reactivity of these metallocarbene precursor have been efficiently utilized in our lab for the carbenylative functionalization of o-vinylaniline/phenol derivatives, multisubstituted allylation of arenes and annulation reactions.[3] In addition, we are also studying their asymmetric approach with suitable chiral catalyst. In this presentation, our efforts on the catalytic functionalization of metallocarbenes and their asymmetric version will be discussed.



References and Notes:

1. a) Doyle, M. P. *Chem. Rev.* **1986**, 86, 919; b) Davies, H. M. L.; Moron, D. *Chem. Soc. Rev.* **2011**, 40, 1857.
2. A) Anbarasan, P.; Yadagiri, D.; Rajasekar, S. *Synthesis* **2014**, 46, 3004; b) Yadagiri, D.; Anbarasan, P. *Chem. Rec.* **2021**, 21, 3872; c) Akter, M.; Rupa, K.; Anbarasan P. *Chem. Rev.* **2022**, accepted.
3. a) Yadagiri, D.; Reddy, A. C. R.; Anbarasan, P. *Chem. Sci.* **2016**, 7, 5934; b) Reddy, A. C. S.; Choutipalli, V. S. K.; Ghorai, J.; Subramanian, V.; Anbarasan, P. *ACS Catal*. **2017**, 7, 6283; c) Rajasekar S.; Anbarasan, P. *Org. Lett.* **2019**, *21*, 3067; d) Reddy, A. C. S.; Ramachandran, K.; Reddy, P. M.; Anbarasan, P. *Chem. Commun.* **2020**, *56*, 5649; e) Reddy, P. M.; Ramachandran, K.; Anbarasan, P. *J. Catal.* **2021**, *396*, 291; f) Ramachandran, K.; Anbarasan, P. *Chem. Sci.* **2021**, *12* 13442.

Bio-Sketch of Speaker

P. Anbarasan
Professor

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Anbarasan obtained PhD on the enantioselective total synthesis of natural product from Indian Institute of Science, Bangalore with Prof. Kavirayani R. Prasad, in 2007. Subsequently, he held postdoctoral position at Leibniz Institute for Catalysis, Germany as Alexander von Humboldt fellow with Prof. Matthias Beller and University of California, Berkeley, USA with Prof. Dean Toste. He joined the Department of Chemistry, Indian Institute of Technology Madras (IITM) in Dec-2011, where currently he is a Professor of Chemistry.

Research Interest:

- Design and development of asymmetric transformations
- Stereoselective functionalization of metallocarbenes
- Trifluoromethylation and trifluoromethylthiolation
- Synthesis of therapeutically important natural products
- Conversion of biomass and carbon dioxide to chemicals and fuels

Awards and Recognitions:

AVRA Young Scientist Award, 2021 – SwarnaJayanti Fellowship, 2019-20 – CRSI-Bronze Medal, 2020 – Young Scientist Award of the Academy of Sciences, Chennai, 2020 – CRSI-Young Scientist Award, 2019 – ISCB Young Scientist Award, 2017 − NASI-Young Scientist Platinum Jubilee Award, 2016 − Institute Research & Development Award (IRDA) of IIT Madras, 2015-2016 − Young Scientist Medal of the Indian National Science Academy (INSA), 2015 − Associate Member of the Indian Academy of Sciences, Bangalore (2015-2018) − DAE-Young Scientist Research Award − Thieme Chemistry Journals Award-2013 − Alexander-*von*-Humboldt fellowship

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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Unactivated Carboxylic Acids in Catalytic Asymmetric Ring Opening Reactions

Nilanjana Majumdar*
Medicinal & Process Chemistry Division
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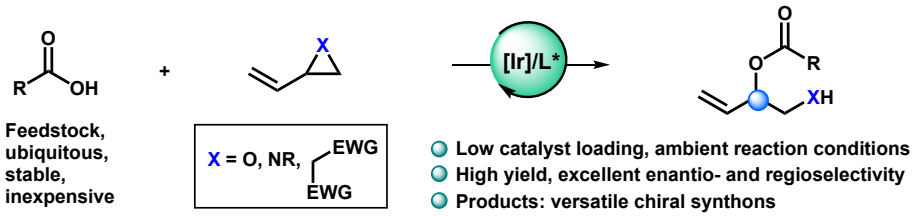
Abstract:
Carboxylic acids are important building blocks as they are widely available, highly stable and inexpensive. They can be excellent choice of substrates in catalytic asymmetric reactions, if utilized properly. However, carboxylic acids are generally not compatible for several important transformations, e.g. carboxylic acids are difficult substrates for nucleophilic reactions as the nucleophile may not survive the acidic conditions. Also, the electrophilicity of the substrate is substantially dominated by its acidic character. On the other hand, carboxylic acids can act as good O-nucleophiles, when there is pre-activation involved to form the carboxylate salt. Free carboxylic acids are quite challenging substrates as nucleophiles because of their extremely poor nucleophilicity. On the other hand, the catalyst is required to be robust enough to resist the acidic as well as oxidizing conditions and take full control of the selectivity in the reaction. Therefore, carboxylic acids are very challenging but intriguing substrates for catalytic asymmetric transformations. Here, efficient and convenient use of free carboxylic acid substrates will be illustrated in catalytic asymmetric ring opening reactions for the preparation of very important class of products that may act as useful chiral synthons.

Figure/Scheme (if any):



References and Notes:

1. Pandit, S.; Adhikari, A. S.; Majumdar, N. "Enantioselective Ring Opening of Alkenyl Oxiranes by Unactivated Carboxylic Acids" (Unpublished results)
2. Adhikari, A. S.; Pandit, S.; Majumdar, N. "Enantioselective Ring Opening of Vinyl Cyclopropanes by Unactivated Carboxylic Acids" (Unpublished results)
3. Kumar, S.; Majumdar, N. "Enantioselective Ring Opening of Vinyl Aziridines by Unactivated Carboxylic Acids" (Unpublished results)

Bio-Sketch of Speaker

Dr. Nilanjana Majumdar
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Dr. Nilanjana Majumdar started her chemistry journey from ***Visva-Bharati University in West Bengal, India***. She completed her undergraduate education there with first class first in B.Sc. (Chemistry Hons.). In 2003, she went to ***IIT Kharagpur*** to pursue Masters. For Ph.D., she moved to ***United States*** in 2006 and worked under the supervision of ***Professor William D. Wulff in Michigan State University***. After graduation in 2012, she moved to ***Tokyo, Japan*** for first postdoctoral experience in ***Professor Masakatsu Shibasaki***'s group with ***JSPS fellowship***. After three years in Japan, she worked in ***Professor Benjamin List***'s group for one year in ***Max-Planck Institut für Kohlenforschung, Germany***. In April, 2018, she joined CSIR-Central Drug Research Institute (CSIR-CDRI), Lucknow as Senior Scientist in Medicinal & Process Chemistry Division.

Awards:

2022 Dr. Mridula Kamboj Award for Drugs, Diagnostics, Vaccines and Related Basic Research-2021
2021 CDRI Incentive Award for Technology 2021, Title: Process for the Preparation of Umifenovir (Antiviral)
2019 DST-SERB Early Career Research Award
2016 Max-Planck Postdoctoral Fellowship (Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany)
2013 Japan Society for the Promotion of Science (JSPS) Fellowship
2012 IMC Fellowship for Postdoctoral Research (Japan)
2006 Doctoral fellowship (Michigan State University, USA)
2005 Council of Scientific & Industrial Research-National Eligibility Test (CSIR-NET) (Conducted by CSIR New Delhi, India)
2003 First Class First in Bachelor of Science (B. Sc. Chemistry Hons.)(Visva Bharati University)

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Dr. Suman De Sarkar

Associate Professor

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

Selected Publications:

1. M. Baidya, D. Maiti, L. Roy*, **S. De Sarkar***, "Trifluoroethanol as a Unique Additive for the Chemoselective Electrooxidation of Enamines to Access Unsymmetrically Substituted NH-Pyrroles" *Angew. Chem., Int. Ed.* **2022**, *61*, e202111679. **(Hot Paper)**
2. M. Baidya, S. Mallick, **S. De Sarkar***, "Regioselective Synthesis of N^2-Aryl 1,2,3-Triazoles via Electro-oxidative Coupling of Enamines and Aryldiazonium Salts" *Org. Lett.* **2022**, *24*, 1274.
3. S. K. Parida, T. Mandal, S. Das, S. K. Hota, **S. De Sarkar*** and S. Murarka* "Single Electron Transfer-Induced Redox Processes Involving *N*-(Acyloxy)phthalimides" *ACS Catal.* **2021**, *11*, 1640.
4. V. Arun, L. Roy*, **S. De Sarkar***, "Alcohols as Fluoroalkyl Synthons: Ni-catalyzed Dehydrogenative Approach to Access Polyfluoroalkyl Bis-indoles" *Chem. Eur. J.* **2020**, *26*, 16649.
5. **S. De Sarkar***, "Remote C−H Functionalization by a Palladium-Catalyzed Transannular Approach" *Angew. Chem., Int. Ed.* **2016**, *55*, 10558.

Awards/Achievements:

- Member of the Early Career Advisory Board of Asian Journal of Organic Chemistry
- Fellow of the Indian Chemical Society
- DSM Science & Technology Award, Netherlands (**2011**)
- D. C. Mukherjee Gold Medal award (**2005**)

Alzheimer's Disease Therapeutics

T. Govindaraju*
Bioorganic Chemistry Laboratory, New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur P.O., Bengaluru-560064, India
(Email: tgraju@jncasr.ac.in)

Abstract:

Alzheimer's disease (AD) is a multifactorial neurological disorder and common form of dementia. There are no fully approved diagnosis and treatment for AD. The production, accumulation, and aggregation of proteins in the human brain are considered as the major hallmarks of the disease. Reactive oxygen species (ROS) are the major sources of biomolecular and mitochondria damage, and oxidative stress in neuronal cells. Oxidative stress, mitochondrial dysfunction, neuroinflammation and microglia contribute significantly to the disease pathogenesis. In this talk, I shall discuss current status of understanding disease mechanisms, and present our multipronged strategies in developing molecular tools to tackle AD.

Bio-Sketch of Speaker

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Bioorganic Chemistry Laboratory
New Chemistry Unit and
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T. Govindaraju received MSc (2000) from Bangalore University and PhD (2006) from the National Chemical Laboratory and Pune University, Pune, India. He carried out postdoctoral research at the University of Wisconsin-Madison, USA (2005–2006) and Max Planck Institute of Molecular Physiology, Dortmund, Germany (2006–2008). His research interests are at the interface of chemistry, biology and biomaterials science, include Alzheimer's disease, peptide chemistry, molecular probes, diagnostic therapy (Theranostics), molecular architectonics, and silk-inspired biomimetics and biomaterials. He has more than 150 publications, >35 patents, and four books to his credit. He has co-founded a startup company (VNIR Biotechnologies Pvt. Ltd. http://vnir.life) to translate many of the inventions from his laboratory including Alzheimer's disease diagnostics. His group has discovered a novel drug candidate with immense potential to treat Alzheimer's disease and is licensed to a biopharma for further development.

Title: Biophysical Aspects of Virus-Membrane Interaction

Author(s) name:Nagma Parveen*
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Abstract:
Viruses are unique pathogen that requires hosts and host cell machinery for their replication. In the early step of replication, the virus particles or virions interact with cell surface[1–3]. In particular, viruses after managing to cross through the cell surface glycocalyx barrier reach to the plasma membrane which is the first and major barrier for viruses to enter inside host cells. Viruses use their surface proteins such as spike proteins to interact with cell membrane receptors. This interaction is specific, dynamic and multivalent in nature [4–6].

I will highlight the ongoing projects of the group focusing on the early-replication steps of virions, in particular, membrane attachment and fusion. I will show the applications of biophysical tools like single-particle fluorescence imaging in combinations with model membrane systems for probing virus-receptor interactions, their multivalent binding and more importantly, the mechanism of their membrane attachment in the native-like environment.

References and Notes:

1. Tang, T. *et al.* A biophysical perspective on receptor-mediated virus entry with a focus on HIV. *Biochim. Biophys. Acta - Biomembr.* **1862**, 183158 (2020).
2. de Vries, E., Du, W., Guo, H. & de Haan, C. A. M. Influenza A Virus Hemagglutinin–Neuraminidase–Receptor Balance: Preserving Virus Motility. *Trends Microbiol.* **28**, 57–67 (2020).
3. Marsh, M. Contents lists available at ScienceDirect BBA - Biomembranes A biophysical perspective on receptor-mediated virus entry with a focus on HIV. (2019).
4. Costello, D. A., Millet, J. K., Hsia, C. Y., Whittaker, G. R. & Daniel, S. Single particle assay of coronavirus membrane fusion with proteinaceous receptor-embedded supported bilayers. *Biomaterials* **34**, 7895–7904 (2013).
5. Parveen, N. *et al.* Competition for Membrane Receptors: Norovirus Detachment via Lectin Attachment. *J. Am. Chem. Soc.* **141**, 16303–16311 (2019).
6. Parveen, N., Borrenberghs, D., Rocha, S. & Hendrix, J. Single viruses on the fluorescence microscope: Imaging molecular mobility, interactions and structure sheds new light on viral replication. *Viruses* **10**, (2018).

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

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Bio-Sketch of Speaker

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- Career Profile, significant awards/achievements and representative publications

2020-on going	Faculty at Indian Institute of Technology Kanpur
2017 – 2019	Postdoctoral fellow at KU Leuven, Belgium
05/2014 – 08/2017	Postdoctoral fellow at Chalmers University of Technology, Sweden
10/2010 – 04/2014	PhD in Natural Sciences Institute of Physical Chemistry, University of Muenster (WWU Muenster), Germany

Representative Publications

1. Julie Janssens, Flore De Wit, Nagma Parveen and Zeger Debyser, Single-Cell Imaging Shows that The Transcriptional State of the HIV-1 Provirus and Its Reactivation Potential Depend on the Integration Site, mBio (ASM), 16 June 2022.

2. Karin Norling, Mattias Sjöberg, Marta Bally, Vladimir P. Zhdanov, Nagma Parveen* and Fredrik Höök*, Dissimilar Deformation of Fluid- and Gel-Phase Liposomes upon Multivalent Interaction with Cell Membrane Mimics Revealed Using Dual-Wavelength Surface Plasmon Resonance, Langmuir, 2022

3. Marta Bally, Stephan Block, Fredrik Höök, Göran Larson, Nagma Parveen and Gustaf E. Rydell, Physicochemical tools for studying virus interactions with targeted cell membranes in a molecular and spatiotemporally resolved context, Analytical and Bioanalytical Chemistry, 413 (29):7157-7178, 2021

4. Parveen, N. *et al.* Membrane Deformation Induces Clustering of Norovirus Bound to Glycosphingolipids in a Supported Cell-Membrane Mimic. *J. Phys. Chem. Lett.* **9**, 2278–2284 (2018).

5. Nagma Parveen, Stephan Block, Vladimir Zhdanov, Gustaf Rydell, and Fredrik Hook, Detachment of Membrane Bound Virions by Competitive Ligand-Binding Induced Receptor Depletion, Langmuir ACS Editors' Choice, 33, 4049-4056, 2017

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

R. Boomi Shankar

Professor

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Career Profile:

Prof. Boomi Shankar obtained his B.Sc. (1996) and M.Sc. (1998) in Chemistry from Madura College affiliated to Madurai Kamaraj University, Madurai, India. He then obtained his Ph.D. from the Indian Institute of Technology, Kanpur, India in 2004 under the supervision of Prof. V. Chandrasekhar. Soon after obtaining his Ph.D. degree in January 2004, he took a short-term postdoctoral position at the University of Illinois at Urban-Champaign, USA. He then worked at the University of Liverpool as a Senior Research Associate for about three years between November 2004 and December 2007. In April 2008, he joined as an Assistant Professor at IIT, Guwahati and later moved to IISER Pune in December 2010. He became an Associate Professor in December 2014 and a full Professor December 2019. The research focus of his group falls in the broad interface of inorganic and materials chemistry with emphasis to synthesis, structure, physical properties and energy applications.

Significant awards/achievements:

- Bronze medal of the Chemical Research Society of India, 2022.
- Science and Technology Award for Research from the Science and Engineering Research Board, India (SERB-STAR), 2021.
- Life Fellow, Indian Chemical Society, 2022.

Representative publications:

1. *Adv. Funct. Mater.* **2022**, *32*, 2109492 (Review Article)
2. *Chem. Rec.* **2022**, doi.org/10.1002/tcr.20210028 (Review Article)
3. *Angew. Chem. Int. Ed.* **2021**, *60*, 4023-4027
4. *Angew. Chem. Int. Ed.* **2020**, 59, 10368-10373
5. *Angew. Chem. Int. Ed.* **2018**, *57*, 9054-9058

Biomimetic Ion Transport and Encapsulation

Nandita Madhavan*
Department of Chemistry
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Abstract:
Ion transport in cellular membranes is mediated by ion-channel proteins and ion-carriers. The dysfunction of ion-transporters leads to several diseases called channelopathies.[1] Synthetic peptides that mimic the function of natural ion transporters serve as attractive therapeutic agents.[2] Peptides are attractive scaffolds due to their biocompatibility and rich functional group diversity. Our group has developed cyclic and acyclic scaffolds that can be incorporated with ion-inducers to offer high ion-selectivity.[3] We have recently developed lipidomimetic small peptides that combine the amphiphilicity of lipids with the ion-binding ability of peptides to afford highly efficient anion transporters.[4] We have also exploited the ability of peptides to self-assemble to create peptide-polymer conjugate membranes for ion-encapsulation.[5] In the long term, we hope to develop totally synthetic peptide-polymer conjugates for selective ion-encapsulation and transport.

References and Notes:

1. Hille, B. *Ion Channels of Excitable Membranes, 3rd ed*.; Sinauer Associates Inc.: Sunderland, 2001; Chapter 1.
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Bio-Sketch of Speaker

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Recent Picture

Nandita Madhavan got her bachelor's degree in Chemistry from S.I.E.S. College (Mumbai University) and her master's degree from IIT Bombay. She joined the University of Illinois at Urbana-Champaign for her Ph.D., where her research focused on cyclodextrin derivatives for light activated ion transport. Her post-doctoral research at Georgia Institute of Technology involved supported catalysts for asymmetric organic synthesis. She started her independent research career in 2009 at IIT Madras and subsequently moved to IIT Bombay in 2016. Her research group mimics the activity of natural ion channel proteins using small peptides. Her group also develops cost-effective methods for peptide synthesis. Nandita is also associated with NPTEL and the Centre of Teaching and Learning at IIT Bombay.

Exploring photophysical processes in molecules and materials with potential to surpass Shockley-Queisser limit

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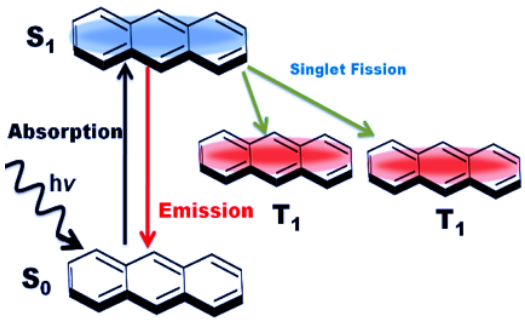
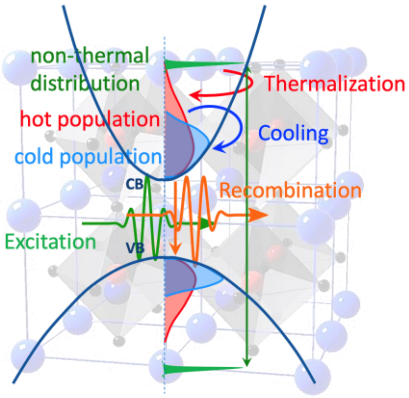
Abstract:
Earth receives several thousand times more energy from the sun than global consumption.[1] Solar cells convert solar energy into electrical energy, known as photovoltaics. New architectures and processes are being explored to surpass the fundamental thermodynamic limit on power conversion efficiency (PCE) of ~33%, i.e., the Shockley-Queisser limit.[2] Singlet fission is a down-conversion process in which an organic chromophore gets excited to its excited singlet state and shares its excitation energy with a ground state chromophore nearby and consequently two triplet excitons are generated.[3] If combined with lower bandgap semiconductor, this procedure can develop three electron-hole pairs, reduce the thermalization loss, and has the potential to increase the maximum PCE to ~44%.[2] Hot carrier solar cells can also boost the efficiency given the excess energy of hot carriers be utilized proficiently.[4] Generally, hot carriers rapidly cool down to band-edge and do not provide sufficient time for extraction. Slowing down the cooling process can lead to efficient extraction.[5] Efficient extraction of hot carriers before thermalization loss can theoretically increase PCE up to ~66% for single-junction solar cells. In this talk, I will discuss our results on observation of singlet fission in anthracene in solution, and hot carrier cooling dynamics in perovskite thin films. Ongoing method development in the group will also be highlighted.





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Bio-Sketch of Speaker

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Profile

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Marie Skłodowska-Curie Fellow (2017-2019) - Cavendish Laboratory, University of Cambridge, UK with Dr. Akshay Rao.
Postdoctoral Scholar (2016 -2017) - Department of Chemistry, University of California, Irvine, USA with Prof. Nien-Hui Ge.
Postdoctoral Fellow (2013-2016) - Department of Chemistry and Biochemistry, University of South Carolina, USA with Prof. Mark Berg.
Ph. D. (2006-2012), Jawaharlal Nehru University, New Delhi with Dr. Sobhan Sen

Awards/Achievements

- Marie Sklodowska-Curie Individual European Fellowship (2017-2019).
- Best Poster award in TSRP - 2012 held in Bhabha Atomic Research Centre, Mumbai, India (2012).
- Best Poster award in FCS - 2011 held in ICGEB, New Delhi, India (2011).
- Best Poster award in FCS - 2010 held in North Eastern Hill University (NEHU), Shillong, India (2010).
- Appreciation Certificate from Prof. Elliot Elson, co-inventor of FCS, for building a fully functional Fluorescence Correlation Spectrometer during FCS - 2009 at Tata Institute for Fundamental Research (TIFR), Mumbai, India (2009).
- National Eligibility Test (NET) in Physics conducted jointly by CSIR and UGC, Govt. of India (2006).

Representative Publications

1. *Non-Equilibrium Carrier Transport in Quantum Dot Heterostructures.* M. Liu, S. D. Verma, Z. Zhang, J. Sung, A. Rao **Nano Lett.** 21, 21, 8945 (2021) Link
2. *Slow Carrier Cooling in Hybrid Pb-Sn Halide Perovskites*. S. D. Verma, Q. Gu, A. Sadhanala, V. Venugopalan, and A. Rao. **ACS Energy Lett.** *4*, 736 (2019) Link
3. *Rate and Amplitude Heterogeneity in the Solvation Response of an Ionic Liquid*. S. D. Verma, S. Corcelli, and M. Berg. **J. Phys. Chem. Lett.** *7*, 504 (2016). Link

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

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Debasis Banerjee graduated with M.Sc. degree in Organic Chemistry from Banaras Hindu University and obtained Ph.D. in organic chemistry from Indian Institute of Technology Kanpur in 2011 with Prof. M. L. N. Rao. Thereafter he moved to Leibniz Institute for Catalysis (LIKAT), Germany for a postdoctoral position with Prof. Matthias Beller (2011-14) and subsequently held another postdoctoral position (2014-2015) at the Stockholm University, Sweden with Prof. Jan-Erling Bäckvall. In 2015, he has accepted a position of Assistant Professor at the Indian Institute of Technology Roorkee (Uttarakhand, India). Currently he is an Associate Professor at the same institute from August 2020. His research interests includes redox-switchable catalysis (RSC) relates to tuning the catalytic activity of a transition metal by designing a suitable ligand in combination with more abundant non-precious metals, enantioselective dual-catalysis, activation of small molecules, perfluoroalkylation technologies and heterogeneous catalysis for sustainable organic transformations.

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

Representative publications:

(a) Vellakkaran, M.; Singh, K.; Banerjee, D. *ACS Catal*., **2017**, *7*, 8152. (b) Singh, K.; Vellakkaran, M.; Banerjee, D. *Green Chemistry*, **2018**, *20*, 2250. (c) Das, J.; Singh, K.; Vellakkaran, M.; Banerjee, D. *Org. Lett*., **2018**, *20*, 5587. (d) Vellakkaran, M.; Das, J.; Banerjee, D. *Chem. Commun.* **2018**, *54*, 12369. (e) Bera, A.; Sk. M.; Singh, K.; Banerjee, D. *Chem. Commun.* **2019**, *55*, 5958. (f) Das, J.; Vellakkaran, M.; Sk. M.; Banerjee, D. *Org. Lett*., **2019** *21*, 7514. (g) Bera, S.; Bera, A.; Banerjee, D.. *Org. Lett.* **2020**, *22*, 6458. (h) Bera, S.; Bera, A.; Banerjee, D. *Chem. Commun.* **2020**, *56*, 6850–6853. (i) Kabadwal, L. M.; Bera, S.; Banerjee, D. *Chem. Commun.* **2020**, *56*, 4777. (j) Bera, A.; Bera, S.; Banerjee, D. *Chem. Commun.* **2021**, *57*, 13042. (k) Kabadwal, L. M.; Bera, S.; Banerjee, D. *Org. Chem. Front.* **2021**, *8*, 7077. (l) Bera, A.; Kabadwal, L. M.; Bera, S.; Banerjee, D. *Chem. Commun.* **2022**, *58*, 10.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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Stereoselective Transformations on Prochiral Cyclic 1,3-diones

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Abstract:
Stereoselective synthesis of highly functionalized carbocycles is an attractive target in synthetic organic chemistry due to their prevalence in several natural products, bioactive compounds and materials. Catalytic enantioselective and diastereoselective desymmetrization of prochiral cyclic 1,3-diones and their derivatives is one of the most efficient and convenient approach to access these scaffolds. In continuation of our interest in the area of desymmetrization, we have developed various stereoselective approaches on prochiral cyclic 1,3-diones for the construction functionalized carbocycles having all-carbon quaternary stereogenic center and details will be presented.

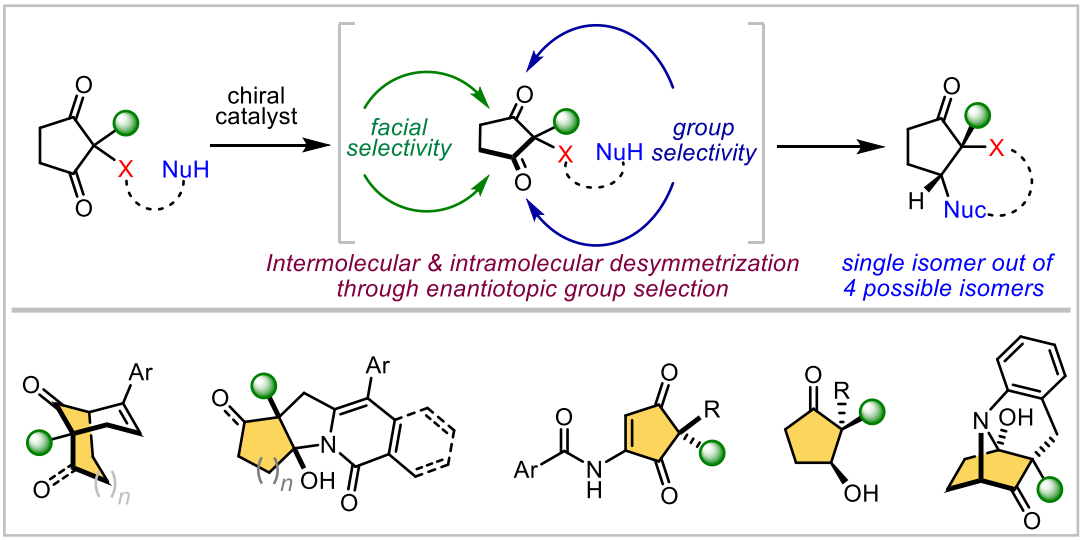

Figure: Stereoselective Transformations on Prochiral Cyclic 1,3-diones

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Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

…Anticipating Tomorrow's Science through Collaborative Ventures

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Rambabu Chegondi received his M.Sc. (2003) degree from University of Hyderabad and completed Ph.D. (2009) in Organic Chemistry from Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad under the supervision of Dr. S. Chandrasekhar. In 2009, he moved to The University of Kansas, USA to work with Prof. Paul R. Hanson as a postdoctoral researcher. After returning from USA, he joined in CSIR-IICT, Hyderabad as CSIR-Pool-Scientist (SRA) in January 2014 to pursue his independent research career. He is currently working as a principal Scientist at Department of Organic Synthesis & Process Chemistry, CSIR-IICT, Hyderabad on the development of new desymmetrization methods for prochiral molecules. His research aimed at the development of new catalytic enantioselective methods and its applications. He received Eli Lilly Asia Best Thesis Award 2009 from Eli Lilly & Company, USA and AVRA-Young Scientist Award-2019.

Representative publications.

1. Jadhav, S. B.; Dash, S. R.; Maurya, S.; Nanubolu, J. B.; Vanka, K.; Chegondi, R. *Nat. Commun.* **2022**, *13*, 854.
2. Gollapelli, K. K.; Patil, V. B.; Vinaykumar, A.; Chegondi, R. *Chem. Sci.* **2021**, *12*, 1544-1550.
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Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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Tuning the Pore Chemistry in Crystalline Frameworks for Improved Separation and Non-redox Fixation of Carbon Dioxide

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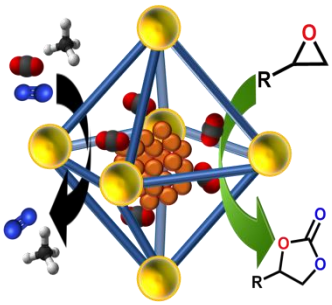
Abstract: The rising concentration of major greenhouse gas, carbon dioxide (CO_2) in the atmosphere is recognized to be the prime contributor to worldwide climate destabilization.[1] Although, post-combustion CO_2 capture is largely considered, this feat is tricky owing to the minimal differences in molecules, present in its main components (CO_2 and N_2).[2] As such, their effective separation requires tailor-made adsorbents with molecule-specific interactions on pore surface. On a similar note, CO_2 valorisation is alternative effective way to get rid of major environmental problem, which embarked research on non-redox fixation of captured CO_2 to value-added chemicals.[3] However, the major flaw of such methodology is the chemical inertness of CO_2 that demands backing of a catalyst. While homogeneous catalyst possesses inherent difficulty of product separation, most heterogeneous catalysis suffer from inadequate activities, toxic solvent assistance, and harsh reaction conditions.

Metal−organic frameworks (MOFs) and covalent organic frameworks (COFs) have caused a renaissance in recent times because of their tunable pore size, structural diversity and wide range of potential applications.[4] In fact, selective CO_2 adsorption and the catalytic CO_2 conversion in these materials are expanding areas of interest. Based on the above facts and challenges, this presentation will mostly cover designed synthesis of robust MOF and COF systems as versatile and emerging class of porous materials for environmental remediation and energy sustainability. In particular, deliberate incorporation of task-specific functionalities through in-situ fabrication and/or post-synthetic modification for improved separation and chemical fixation of CO_2 will be discussed.[5]

Figure/Scheme:



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2. Solomon, S.; Plattner, G. K.; Knutti, R.; Friedlingstein, P. *Proc. Natl. Acad. Sci. U. S. A.* **2009**, *106*, 1704– 9
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4. Guan, X.; Chen, F.; Fang, Q.; Qiu, S. *Chem. Soc. Rev.* **2020**, *49*, 1357– 1384.
5. (a) Seal, N.; Karthick, K.; Singh, M.; Kundu, S.; Neogi, S., *Chem. Eng. J.*, **2022**, *429*, 132301. (b) Seal, N.; Neogi, S., *ACS Appl. Mater. Interfaces*, **2021**, *13*, 55123–55135; (c) Singh, M.; Palakkal, A. S.; Pillai, R. S.; Neogi, S., *J. Mater. Chem. C*, **2021**, *9*, 7142-7153; (d) Kumar, G.; Singh, M.; Goswami, R.; Neogi, S., *ACS Appl. Mater. Interfaces*, **2020**, *12*, 48642–48653; (e) Singh, M.; Solanki, P.; Patel, P.; Mondal, A.; Neogi, S., *Inorg. Chem.* **2019**, *58*, 8100–8110.

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

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Dr. Subhadip Neogi received Ph.D. from I.I.T. Kanpur in 2008 under the supervision of Prof. P. K. Bharadwaj. After spending a year as NRF Post-doctoral Fellow with Prof. Barbour at the Stellenbosch University, he joined the group of Prof. Schmittel, University of Siegen, first as Humboldt Post-Doctorate and later as a DFG Fellow. Before joining CSIR-CSMCRI, he worked as an Assistant Professor at the Galgotias University. Dr. Neogi has been working in porous materials for nearly fifteen years. His research interest includes metal-organic frameworks and covalent organic frameworks for gas separation, monitoring of toxic chemicals, and heterogeneous catalysis. He published more than sixty research papers in international journals, and authored three book chapters.

Representative publications:

1. R. Goswami, K. Karthick, S. Das, S. Rajput, N. Seal, B. Pathak, S. Kundu, **S. Neogi** *ACS Appl. Mater. Interfaces*, **2022**, *14*, 29773-29787**.**
2. **R. Goswami**, B. D. Bankar, S. Rajput, N. Seal, R. Pillai, A. V. Biradar, **S. Neogi** *J. Mater. Chem. A*, **2022**,*10*, 4316-4332.
3. N. Seal, K. Karthick, M. Singh, S. Kundu, **S. Neogi** *Chem. Eng. J.*, **2022**, *429*, 132301.
4. N. Seal, **S. Neogi** *ACS Appl. Mater. Interfaces*, **2021**, *13*, 55123–55135.
5. G. Kumar, R. S. Pillai, N. H. Khan, **S. Neogi** *Appl. Catal. B-Environ.*, **2021**, *292*, 120149.
6. R. Goswami, S. Das, N. Seal, B. Pathak, **S. Neogi** *ACS Appl. Mater. Interfaces*, **2021**, *13*, 34012-34026.

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Supratim Banerjee received his MS and PhD degrees at the Indian Institute of Science, Bangalore, India. Following two Post-Doctoral stays at the University of Regensburg and University of Duisburg-Essen (both in Germany), he joined the Indian Institute of Science Education and Research (IISER) Kolkata, India in 2016 and is currently holding the position of Associate Professor in the Department of Chemical Sciences. His research interests include luminescent supramolecular polymers, photo-responsive self-assembled materials, small molecule and multivalent luminescent sensors for bio-analytes, host-guest chemistry and artificial light harvesting systems.

Recent Publications:

1. "Multicolor-Luminescence including White Light by Photomodulation of Supramolecular Assemblies in Aqueous Media" S. K. Bhaumik and S. Banerjee*, *ACS Appl. Mater. Interfaces* **2022** (Accepted).
2. "Cucurbituril Based Luminescent Materials in Aqueous Media and Solid State" S. K. Bhaumik, R. Biswas and S. Banerjee* *Chem. Asian. J.* **2021**, *16*, 2195-2210.
3. "A Remarkable Fluorescence Quenching Based Amplification in ATP Detection through Signal Transduction in Self-assembled Multivalent Aggregates", R. Biswas, S. Naskar, S. Ghosh, M. Das,* and S. Banerjee*, *Chem. Eur. J.* **2020**, *26*, 13595-13600.
4. "High affinity heparin detection by multivalent supramolecular polymers through aggregation induced emission" S. K. Bhaumik, Y. S. Patra and S. Banerjee*, *Chem. Commun*. **2020**, *56*, 9541-9544.
5. "Tunable Multi-color Luminescence from a Self-assembled Cyanostilbene and Cucurbit[7]uril in Aqueous Media" S. K. Bhaumik and S. Banerjee*, *Chem. Commun*. **2020**, *56*, 655-658.

Rethinking Solutions for Healthcare Technologies

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Abstract:

Among myriad of health issues of global populace today, the problems associated with better means of diagnosis, and repair and regeneration of organs, bones, cartilages, etc. remain a big challenge. The prospect of using nanoscience and nanotechnology as a tool to answer questions arising out of these healthcare issues are exciting and form the basis of this talk. Nanostructures, due to their similar size scale as bio-macromolecules and cellular components, provide an unprecedented opportunity to target and potentially modulate important biological processes. Some of the key nanotechnology based scientific and technological contributions from our laboratory that will impact future healthcare strategies impacting disease diagnostics, better therapeutics delivery and tissue engineering will be discussed. Briefly, examples illustrating how knowledge of chemical science & nanotechnology has enabled us to develop platform technologies for easy quantification of cell growth, migration and disease progression along with nano-based solutions from our lab for improving drug delivery, wound healing and tissue engineering will be discussed.

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Neetu Singh obtained her Bachelors and Masters degrees from University of Mumbai and her doctoral degree in chemistry from Georgia Institute of Technology, Atlanta, USA. She obtained her postdoctoral training at the Harvard-MIT Division of Health Sciences and Technology, USA. Prof. Singh returned to India and joined IIT Delhi as an Assistant Professor in the Center for Biomedical Engineering in 2014.

In her current program at IITD, she is establishing a research program that explores systematic probing into nanomaterials biological activity and formulates "design rules" for developing nanosystem for specific bio-medical & healthcare applications. Her group at IIT Delhi is integrating concepts and skills from chemistry, materials science, and biology to design nano-structured materials with enhanced functionalities for applications in biomedical implants, disease diagnostics, tissue engineering and regenerative medicine.

Her scientific contribution has been recognized by several awards and honors. She is the recipient of "Innovative Young Biotechnologist award 2013" by Department of Biotechnology (DBT), India. In 2019, she received the Veena Arora young researcher award by IIT Delhi, which recognizes best research contributions at IIT Delhi by faculty below 40 years. She is the receipt of NASI-SCOPUS young Scientist award for "Women-in Science"-2019; DBT's Janaki Ammal Young scientist -2021 and Science and Engineering Research Board (SERB)-India, POWER Fellow 2021. She is also a mentor for an IITD start-up, "Kriya-Labs", that is bringing valorization to agro waste by technological solutions.

She is also an editorial advisory board member of the journal Bioconjugate Chemistry (a pioneering publication of American Chemical Society) and a new Springer journal - In Vitro Models.

Folding of aromatic polyamides into a rare intrachain β-sheet type structure and their remarkable selectivity in guest encapsulations

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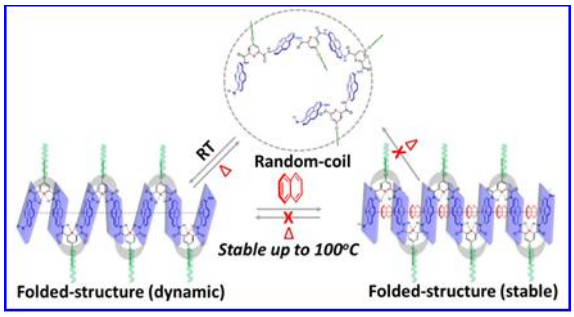
Abstract:
During the last two decades, synthetic macromolecules have been successfully folded into various types of secondary structures by following biological principles. Despite significant advancement, owing to their intrinsic aggregation tendency, mimicking the β-sheet structure is relatively rare. Since the pioneering work by Hamilton and co-workers in the late 90s,[1] a large number of aromatic oligoamides based on heterocycles and benzene-derivatives have been designed and synthesized for folding studies. Among various folded structures, helix, planar-sheet, and zigzag structures are the most common secondary structures that have been observed so far.
In my presentation, I will demonstrate the design of a polymer and the underlying principles for mimicking β-sheet structure. To this objective, a pair of periodically-grafted clickable aromatic polyamides have been designed and their propensity to fold into a βsheet-like structure has been studied experimentally and by using computational studies. Among the two polymer chains, the polymer comprises both intramolecular H-bonding as well as π-stacking motifs readily fold into a βsheet-like secondary structure. However, the other polymer was structurally identical to the previous one except for the intramolecular H-bonding motifs, assuming random-coil conformations under similar experimental conditions. In addition to demonstrating the role of the H-bonding and π-stacking interactions in effecting βsheet-like folding, the reinforcement of this secondary structure through host-guest interactions and their selectivity for the same will also be demonstrated. Moreover, few preliminary studies have been conducted to demonstrate their potential applications as through-space electron conducting materials.[2]



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Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

Dr. Raj Kumar Roy
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Dr. Raj Kumar Roy received both his MS (2008) and Ph.D. degree (2012) from IISc Bangalore in polymer chemistry under the supervision of Professor S Ramakrishnan. His doctoral research focused on synthetic polymer chemistry more precisely on hyperbranched polymers. He did postdoctoral research (2012-2015) in Strasbourg working on sequence-controlled and sequence-defined polymers synthesis with Professor Jean-Francois Lutz and subsequently moved to Nagoya University, Japan as a VBL research fellow and JSPS postdoctoral fellow (2015- 2017) and worked in the area of helical polymers with Professor Eiji Yashima. He joined IISER Mohali in 2017 as an Assistant professor. His current research focused on precision polymer synthesis, conformational-control phase separation of block copolymers, organic ferroelectric materials, foldamers, etc. Dr. Roy was awarded a SERB early carrier grant in 2019.

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

…Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

Ravi P. Singh
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- **Post-Doctoral Fellow:** Harvard University, **Prof. E. J. Corey** (Nobel Laureate), 2005-2007.
- **Post-Doctoral Fellow:** Brandeis University, Prof. Li Deng, 2007-2011**.**
- **Senior Scientist:** National Chemical Laboratory, Pune, 2011–2013.
- **Assistant Professor:** Academy of Scientific and Innovative Research, New Delhi, 2011–2013.
- **Assistant Professor:** Indian Institute of Technology Delhi, 2013-2016.
- **Associate Professor:** Indian Institute of Technology Delhi, 2016-2021.
- **Professor:** Indian institute of Technology, Delhi, 2021- Present.

Chiral Catalysis and Synthesis Laboratory (CCSL)

CCSL is a synthetic chemistry laboratory aimed towards achieving the synthesis of small molecules via contemporary approaches in organic chemistry. Our research efforts are geared towards designing, synthesizing and optimizing catalysts (organo and acid-base) for enantioselective transformations for the synthesis of a small molecule. We are also focusing on transition metal catalyzed activation of inert C-H bond and converting it to a more resourceful functional group. Further, the synthetic methods (including asymmetric) developed at CCSL are extended towards the total synthesis of structurally fascinating and biologically active molecules.

De novo Design of Lipopeptide-based Fusion Inhibitor as Potential Broad-spectrum Antiviral

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Indian Institute of Science Education and Research Kolkata
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Abstract:
The entry of enveloped viruses requires the fusion of viral and host cell membranes. An effective fusion inhibitor aiming at impeding such membrane fusion may emerge as a broad-spectrum antiviral agent against a wide range of viral infections. Mycobacterium survives inside the phagosome by inhibiting phagosome-lysosome fusion with the help of a coat protein coronin 1. Structural analysis of coronin 1 and other WD40-repeat protein suggest that the trp-asp (WD) sequence is placed at a distorted β-meander motif (more exposed) in coronin 1. The unique structural feature of coronin 1 was explored to identify a simple lipo-peptide (Myr-WD), and branched lipopeptide (Myr-D$(WD)_2$), which effectively inhibits membrane fusion by modulating the interfacial order, water penetration, and surface potential. The mycobacterium-inspired lipopeptides were successfully tested to combat type 1 influenza virus (H1N1, H9N2), murine coronavirus, and human coronavirus (HCoV-OC43) infections as a 'potential broad-spectrum' antiviral agent.

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1. Sardar, A.; Lahiri, A.; Kamble, M.; Mallick, A.I.; Tarafdar, P.K., *Angew. Chem. Int. Ed.* **2021**, *60*, 6101-6106.

Bio-Sketch of Speaker

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Career Profile, significant awards/achievements and representative publications

PhD (2010), University of Hyderabad.
NIH-Postdoctoral Fellow (2010-12), University of North Carolina at Chapel Hill.
Alexander von Humboldt Fellow (2013-14), Max-Planck Institute for Biophysical Chemistry.
DST-Inspire Faculty Fellow (2014-15), Saha Institute of Nuclear Physics.
Assistant Professor (2015-2021), Indian Institute of Science Education and Research Kolkata.

Research Interests: Antivirals, Biomaterials, Organic synthesis in water

Representative Publications:

1) Mandal et al., Membrane Transport Inspired Hydrolysis of Non-activated Esters at Near Physiological pH. *Chem. Commun.*, 57, 11088, **2021**.

2) Sardar et al., Translation of Mycobacterium Survival Strategy to Develop a Lipo-peptide based Fusion Inhibitor. *Angew. Chem. Int. Ed.*, 60, 6101, **2021**.

3) Sardar et al., A headgroup linker perturbs pKa via acyl chain migration: designing base-labile supramolecular assemblies. *Chem. Commun.*, 54, 4282, **2018**.

Title: Towards a Unified Stereochemical Model for Metal Catalyzed X-H Insertion Reactions

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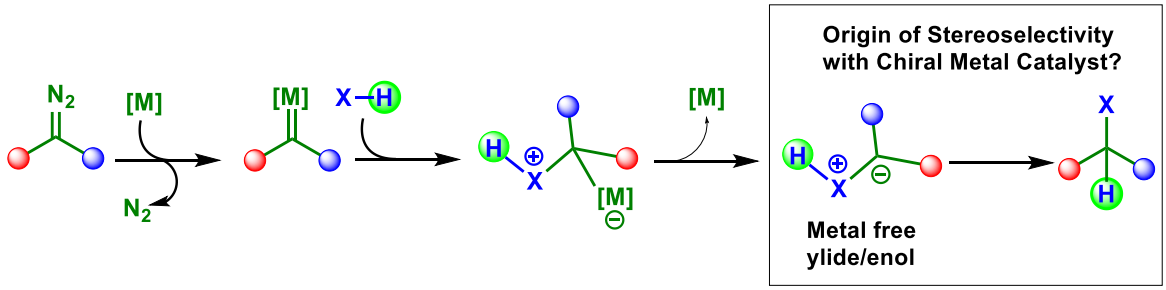
Abstract:
Metal catalyzed carbene insertion into X-H (X=O, N, S, C(sp^2), *etc.*) bonds presents an elegant strategy for C-X bond formation.[1] The general mechanism either involves the nucleophilic attack of the X-H substrate on the metallocarbene intermediate resulting in a metal ylide or a concerted pathway.[2] In a seminal computational study in 2009, Yu and coworkers reported that for an O-H insertion reaction catalyzed by Rh and Cu, different mechanistic pathways are followed.[3] The formation of a metal-free enol was attributed to the lack of successful asymmetric reactions for Rh that led to the advent of cooperative catalytic systems. Surprisingly, there have been reports that utilize a single chiral catalyst for achieving high levels of enantioselectivity. However, with the existing metal-free enol pathway, the origin of enantioselectivity cannot be explained. In the talk, I will discuss the mechanisms of Fe, Rh and Pd catalyzed transformations using DFT methods and show how these three catalysts follow a common pathway involving an enol intermediate and then discuss a new and unified stereochemical model.[4]



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2) (a) Manoj, N.; Jindal, G. *Chem. Commun.* **2021**, *57*, 11370. (b) Balhara, R.; Chatterjee, R.; Jindal, G. *Phys. Chem. Chem. Phys.* **2021**, *23*, 9500.
3) Liang, Y.; Zhou, H.; Yu, Z.-X. *J. Am. Chem. Soc.* **2009**, *131*, 17783.
4) Balhara, R. Jindal, G. *J. Org. Chem.* **2022**, *87*, 7919.

Bio-Sketch of Speaker

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Garima completed her undergraduate and postgraduate studies in Chemistry from the University of Delhi. She moved to IIT Bombay to pursue her graduate studies with Prof. Sunoj. In 2015, she joined the group of Prof. Warshel at the University of Southern California as a postdoctoral fellow. She started her independent research career as an assistant professor at IISc Bangalore in March 2019. Her research group is interested in understanding the mechanisms of enzyme and small molecules catalyzed carbene insertion reactions. She was awarded the Rekha Rao Young Investigator Award in 2021.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

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Career Profile

Professor at IISER Kolkata, 2018 - present
Associate Professor at IISER Kolkata, 2013-2018
Assistant Professor at IISER Kolkata, 2009-2013

Significant awards/achievements

Marie Curie Fellow 2006-2008
WRDF Strategic award Research Fellow 2008
Best Thesis award by IISc, Bangalore
University medal for first position in M.Sc.(Chem)

Representative publications

1. Chakraborty, A‡**;** Roy, S‡; Chakraborty, M.P; Roy, Shantanu S; Purkait, K; Koley, T.S; Das,; Acharya, M; Mukherjee, A*. Cytotoxic Ruthenium(II) Complexes of Pyrazolylbenzimidazole 2 Ligands That Inhibits VEGFR2 Phosphorylation. *Inorg. Chem.* **2021**, 60, 18379–18394
2. Mukherjee, A‡; Koley, T.S‡; Chakraborty, A; Purkait, K; Mukherjee, A*. Synthesis, structure and Cytotoxicity of N,N and N,O coordinated Ru(II) complexes of 3-aminobenzoate Schiff bases against Triple-negative breast cancer. *Chem-Asian J.* **2021,** 10.1002/asia.202100917. (*Special Edition for IISER Pune and IISER Kolkata*)
3. Chatterjee**,** R‡**;** Bhattacharya**,** I‡**;** Roy, S; Purkait, K; Koley, TS ; Gupta, A; Mukherjee, A*. Synthesis, Characterization and Cytotoxicity of Morpholine-Containing Ru(II)-p-cymene complexes. *Inorg. Chem.* **2021,** *60*, 12172-12185.
4. Maji, M; Bhattacharya, I; Acharya, S; Chakraborty, M.P; Das, R ; Gupta, A; Mukherjee, A*. Hypoxia Active Platinum(IV) Prodrugs of Orotic Acid Selective to Liver Cancer Cells. *Inorg. Chem.* **2021**, 60, 4342-4346.
5. Chakraborty, M.P‡; Bhattacharyya S‡; Roy S; Bhattacharya, I; Das, R*; Mukherjee, A*. Selective targeting of the inactive state of hematopoietic cell kinase (Hck) with a stable curcumin derivative. *J. Biol. Chem.* **2021**, *229*, 100449.
6. Acharya, S; Ghosh, S; Maji, M; Ajmal Roshan U.P; Singh, S*; Mukherjee, A*. Inhibition of 3D colon cancer stem cell spheroids by cytotoxic Ru(II)-p-cymene complexes of mesalazine derivatives. *Chem. Commun.* **2020**, *56*, 5421-5424.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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Synthetic Pigments for Applications in PDT of Cancer

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Indian Institute of Technology Gandhinagar, Palaj Campus, Gandhinagar- 382355, India

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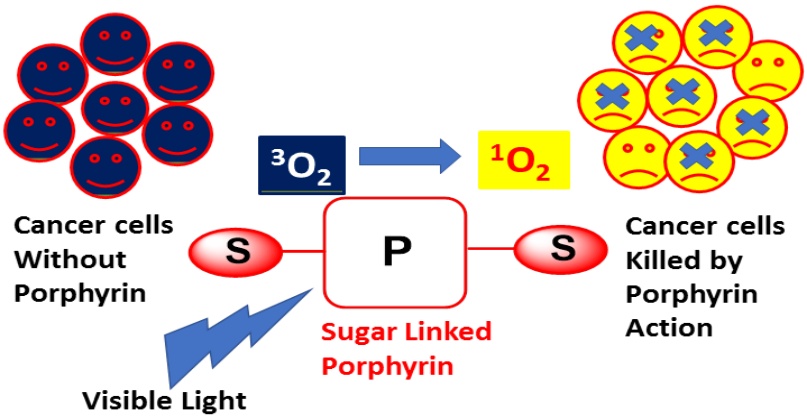
Abstract:

Porphyrin and BODIPY are well known fluorescent dyes, which are used as theranostic agents in magnetic resonance imaging (MRI) and photo-dynamic therapy (PDT) of cancers [1]. The substitution of other chromophores viz. carbazole/ triphenylamine/ phenothiazine on the molecular skeleton can be beneficial to fine-tune the spectral properties of these dyes [2]. The attachment of thio-hexose sugars on the *meso*-positions can yield water soluble derivatives; such thio-glycosylated porphyrins/BODIPYs are highly desirable for optical imaging and can be targeted towards cell receptors rich in lectins for PDT application. Our group at IIT Gandhinagar, is involved in the synthesis and biological applications of porphyrins [3], BODIPYs [4] and dipyrrinato metal-complexes [5]. In this talk, we present the synthesis, photophysical properties and PDT studies of thio-glycosylated BODIPYs and porphyrins containing electron rich bulky aromatic groups on their *meso*-positions.

Figure/Scheme (if any):



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1. (a) Das, S.; Gupta, I.; *J. Porphyrins & Phthalocyanines* **2019,** *23***,** 367-409; (b) Gupta, I.; Praseetha, E. K.; *Front. Chem.* **2019**, *7*, 841.

2. (a) Pandey, V.; Raza, M. K.; Joshi, P.; Gupta, I.; *J. Org. Chem.* **2020**, *85*, 6309-6322; (b) Das, S.; Bhat, H. R.; Balsukuri, N.; Jha, P. C.; Hisamune, Y.; Ishida, M.; Furuta, H.; Mori, S.; Gupta, I.; *Inorg. Chem. Front.* **2017**, *4*, 618-638.

3. (a) Praseetha, E. K.; Pandey, V.; Raza, M. K.; Mori, S.; Gupta, I.; *Bioorg. Chem.* **2019**, *91*, 103139; (b) M. Vedamalai, D. Kedariya, R. Vasita, I. Gupta, *Sensors and Actuators B: Chem.* **2018**, *263*, 137-142.

4. N. Manav, Praseetha, E. K.; Ishida, M.; Mori, S.; Yasutake, Y.; Fukatsu, S.; Furuta, H.; Gupta, I.; *Dalton. Trans.* **2019**, *48*, 2467-2478; (b) N. Manav, Lone, M. Y.; Raza, M. K.; Chavda, J.; Mori, S.; Gupta, I.; *Dalton. Trans.* **2022**, *51*, 3849-3863.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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Recent Picture

Career Profile: Iti Gupta obtained PhD in Chemistry from Indian Institute of Technology Bombay, India. She received JSPS-fellowship from Japan and did postdoctoral research at Kyushu University, Fukuoka where she worked on expanded porphyrins. Later she joined BITS-Pilani KKBirla Goa campus as faculty in Chemistry (2007-2009). She moved to Gandhinagar in July 2009; currently, she is Associate Professor at Indian Institute of Technology Gandhinagar. Her research group is engaged in the synthesis and computational studies of variety of "Synthetic Pigments" like porphyrins, corroles, BODIPYs, metal-dipyrrinates. The Porphyrin and BODIPY derivatives are very promising candidates for NIR (near infra-red) dyes due to their strong absorption and emission properties around 500-900 nm range. NIR light can penetrate non-invasively deep into biological tissue as compared to UV-vis light; thus NIR fluorescent dyes have important roles in bioimaging, chemosensing, ROS generation and photo-dynamic therapy (PDT). Also, BODIPYs and Porphyrins can be employed as fluorescent tag for biomolecules and as photosensitizers in cancer therapy. She has authored/co-authored more than 50 research papers in refereed international /national journals (H-index 22). She is serving as Associate Editor in ***Photocatalysis and Photochemistry*** (specialty section of ***Frontiers in Chemistry***).

Representative Publications:

1. N. Manav, M. Lone, M. K. Raza, J. Chavda and S. Mori, and I. Gupta* *Luminescent Iridium(III) Dipyrrinato Complexes: Synthesis, X-ray Structures, DFT and Photocytotoxicity Studies of Glycosylated Derivatives*, ***Dalton Transactions***, 51, 3849-3863, **2022.** DOI: 10.1039/D1DT04218A.
2. V. Pandey**,** M. K. Raza**,** M. Sonawal and I. Gupta***** *BODIPY based red emitters: Synthesis, computational and biological studies*, ***Bioorganic Chemistry***, 106, 104467, **2021.** Doi: 10.1016/j.bioorg.2020.104467**.**
3. V. Pandey**,** M. K. Raza**,** P. Joshi and I. Gupta* *Synthesis of Water-Soluble Thioglycosylated trans-A2B2 Type Porphyrins: Cellular Uptake Studies and Photodynamic Efficiency*, ***The Journal of Organic Chemistry***, 85, 6309-6322, **2020.** DOI: 10.1021/acs.joc.9b03491
4. N. Manav, Praseetha E. K**.,** M. Ishida, S. Mori,Y. Yasutake, S. Fukatsu, H. Furuta, and I. Gupta* *Phosphorescent Rhenium-Dipyrrinates: Efficient Photosensitizers for Singlet Oxygen Generation*, ***Dalton Transactions***, *48, 2467-2478*, **2019.** DOI:org/10.1039/C8DT04540B
5. S. Das, H. R. Bhat**,** N. Balsukuri, P. C. Jha,Y. Hisamune, M.Ishida, H. Furuta, S. Mori and **I**. Gupta***;** *Donor–acceptor type A2B2 porphyrins: synthesis, energy transfer, computational and electrochemical studies;* ***Inorganic Chemistry Frontiers***, 4, 618-638, **2017.** doi.org/10.1039/C6QI00558F
6. M. Vedamalai, V. G. Krishnakumar, S. Gupta, S. Mori, I. Gupta* *Synthesis and characterization of styryl-BODIPY derivatives for monitoring in vitro Tau aggregation*, ***Sensors and Actuators B: Chemical***, 244, 673–683, **2017.** DOI10.1016/j.snb.2016.12.104

Synthetic Studies Towards Dibenzobicyclo[3.2.1]octadienone Containing Natural Products

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Abstract:
The dibenzobicyclo[3.2.1]octadienone scaffold, which has been found in naphthocyclinones, engelharquinones, rubialatin A, etc., (Figure 1).[1] Most of these natural products exhibit a wide variety of biological activities such as antibacterial, antitumor, antifungal, and cytotoxic properties. We have developed a mild, transition-metal-free, synthetic strategy to access the challenging dibenzobicyclo[3.2.1]octadienone scaffolds by aryne insertion reaction with 2-keto-1,3-indandiones.[2] The foremost advantages of the protocol are direct access to 4 to 5 fused rings containing dibenzobicyclo[3.2.1]octadienone scaffolds as well as the tolerance of various functional groups. Application of this strategy has been demonstrated to the synthesis 6/6/5/6/6 dibenzobicyclo[3.2.1]octadienone skeleton of a rubialatin A. The simple reaction conditions and flexible synthetic strategy offer a unique path to the total synthesis of unaccomplished targets, (α-δ)-naphthoquinones, and other related natural products. ^{1}H NMR experimental studies suggested this reaction proceeds through benzocyclobutane formation followed by a 7-membered carbocycle ring.[2]

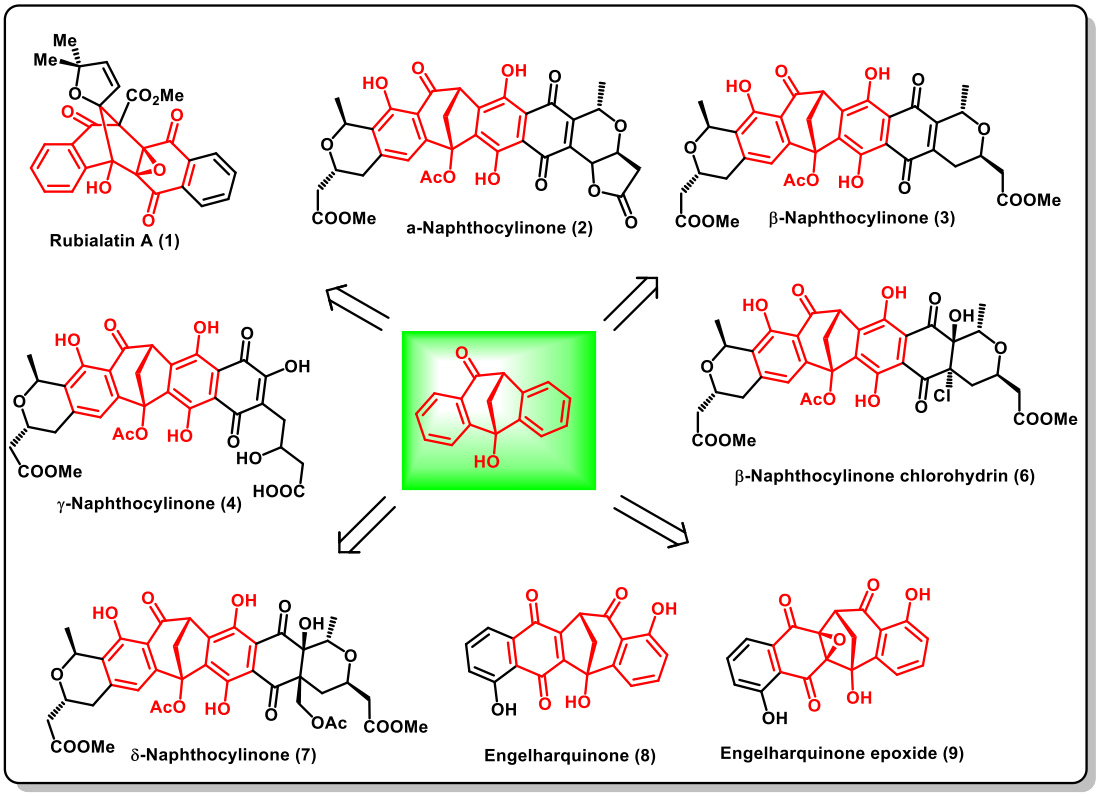

Figure 1: A few natural products bearing dibenzobicyclo[3.2.1]octadienone scaffold

References and Notes:

(1) a) Kamo, S.; Kuramochi, K.; Tsubaki, K. *Tetrahedron Letters* **2018**, 59, 224–230; b) Fernandes, R. A.; Patil, P. H.; Chaudhari, D. A. *Eur. J. Org. Chem.* **2016**, 2016, 5778–5798;

(2) Hazra, G.; Mishra, G.; Dandela, R.; Thirupathi, B. *The Journal of organic chemistry* **2022**., DOI: 10.1021/acs.joc.2c00340

Bio-Sketch of Speaker

Name Dr. Thirupathi Barla
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1. A Method to Access Highly Functionalized Dibenzobicyclo[3.2.1]octadienones: Application to the Construction of the 6/6/5/6/6 Carbon Skeleton of Rubialatin A.; Hazra, G.; Mishra, G.; Dandela, R.; **Thirupathi, B.*** *The Journal of Organic Chemistry*, **2022**, DOI: 10.1021/acs.joc.2c00340 (*Selected for journal front cover page*).

2. Total synthesis of proposed elgonene C and its (4*R*,5*R*)-diastereomer.; Mandal, S.; **Thirupathi, B.*** *Org. Biomol. Chem.* **2022**. DOI: 10.1039/D2OB00094F (*Highlighted on journal front cover page*).

3. Strategies for the Construction of γ-Spirocyclic Butenolides in Natural Product Synthesis.; Sudip Mandal, **Thirupathi, B.*** *Org. Biomol. Chem.* **2020**,*18*, 5287-5314.

Raja Shunmugam

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Raja Shunmugam received his bachelor's degree in 1994, a master's degree in 1996 from V. O. C. College, Manonmaniam Sundaranar University, Tamil Nadu. He received his Ph. D. from the Indian Institute of Technology Madras under Professor R. Dhamodharan. He then joined Professor Gregory N Tew's laboratory in the Polymer Science and Engineering Department at the University of Massachusetts, Amherst as a postdoctoral research associate from 2003 to August 2008.

From September 2008 to 2013, he was an Assistant Professor in the Department of Chemical Sciences at the IISER-Kolkata. From January 2014 to September 2018, he was an Associate Professor in the Department of Chemical Sciences at the IISER-Kolkata. He was the Head of the Department from February 2014 to March 2016. From October 2018 onwards, he has been a full Professor in the Department of Chemical Sciences.

He was a recipient of the prestigious Ramanujan Fellowship from the Department of Science and Technology, Government of India. He received the Joint Runner-Up award in the 6th NATIONAL AWARD FOR TECHNOLOGY INNOVATION under the Polymeric Materials category, 20 January 2016, for the Arsenic sensing work. He also received the Joint Winner Award in the 7th NATIONAL AWARD FOR TECHNOLOGY INNOVATION under the Polymeric Materials category, 01 March 2017, for developing a sensor for nerve agents. In 2018, his group received the Joint Runner-Up award in the National Award for Technology Innovation under the polymeric Materials category for developing New Polymer for Drug Delivery application. Raja is the recipient of the coveted NASI-Reliance Industries Platinum Jubilee Award for the year 2019.

Under his guidance, 14 Ph.D. students already graduated, and currently, 7 students are undergoing their Ph.D. degrees. Raja has published 107 International peer-reviewed publications, six Book Chapters, and one book. He also owns five patents to his credit.

Mirror-image protein as a potential antimalarial therapeutic

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Abstract:

Apical membrane antigen 1 (*Pf*AMA1) and rhoptry neck protein 2 (*Pf*RON2) are two key *Plasmodium falciparum* proteins responsible for the moving junction formation that triggers malaria parasite entry into red blood cells. Identifying a suitable small protein to interfere with the interactions between AMA1 and the extracellular domain of RON2 would be an ideal strategy to snap off the junction formation, which, in turn, will stop the invasion process. We are using a unique combination of 'chemical protein synthesis' and 'mirror-image phage display' to systematically identify mirror-image protein molecules (consisting of all D-amino acids and glycine) that will have potential to interfere with the *Pf*AMA1-*Pf*RON2 interactions. Mirror-image proteins are resistant to proteolysis and less immunogenic. Therefore, a suitably engineered mirror-image protein molecule would be superior to a conventional natural peptide/protein as a candidate antimalarial therapeutic.

Bio-Sketch of Speaker

Kalyaneswar Mandal
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Kalyaneswar Mandal is a Reader of Chemistry and Chemical Biology at the Tata Institute of Fundamental Research (TIFR) Hyderabad. He received his Ph.D. from IIT Bombay in organic chemistry. After completing his Ph.D. he worked at The University of Chicago, first as a Postdoctoral Fellow and later as a Research Professional Associate (Research Faculty position). In 2016, he joined the TIFR faculty at Hyderabad. He is a recipient of the DBT/Wellcome Trust India Alliance Intermediate Fellowship award. Dr. Mandal's research focuses on the chemical protein synthesis combined with biophysical methods to elucidating and controlling the molecular basis of protein function.

Selected Publications:

1. Sinha S,§ Biswas A,§ Mondal J* and **Mandal K* (2021)** Computational and experimental studies of Plasmodium falciparum protein *Pf*AMA1 domain-II loop dynamics: implications in *Pf*AMA1-*Pf*RON2 binding event. ***bioRxiv***, doi:https://doi.org/10.1101/2021.10.10.463826.
2. Mannuthodikayil J, Sinha S, Singh S, Biswas A, Ali I, Mashurabad PC, Tabassum W, Vydyam P, Bhattacharyya, MK and **Mandal K* (2021)** A chimeric peptide inhibits red blood cell invasion by Plasmodium falciparum with hundredfold increased efficacy. ***bioRxiv***, doi:https://doi.org/10.1101/2021.09.28.462119.
3. Das A, Yadav A, Gupta M, Purushotham R, Terse VL, Vishvakarma V, Singh S, Nandi T, Banerjee A, **Mandal K**, Gosavi S, Das R, Ainavarapu SRK and Maiti S **(2021)** Rational design of protein-specific folding modifiers. ***Journal of the American Chemical Society***, 143: 18766-18776.
4. Sarkar A and **Mandal K* (2021)** Repurposing an Antiviral Drug against SARS-CoV-2 Main Protease. ***Angewandte Chemie, International Edition*** **(Highlight)** 60: 23492-23494.
5. Kar A, Mannuthodikayil J, Singh S, Biswas A, Dubey P, Das A and **Mandal K* (2020)** Efficient Chemical Protein Synthesis using Fmoc-Masked N-Terminal cysteine in Peptide Thioester Segments. ***Angewandte Chemie, International Edition*** 59:14796-14801.
6. Mannuthodikayil J, Singh S, Biswas A, Kar A, Tabassum W, Vydyam P, Bhattacharyya, MK and **Mandal K*(2019)** Benzimidazolinone-free peptide o-aminoanilides for chemical protein synthesis. ***Organic Letters*** 21:9040-9044.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Insights into the biosynthesis of bottromycin: A promising ribosomal antibiotic natural product

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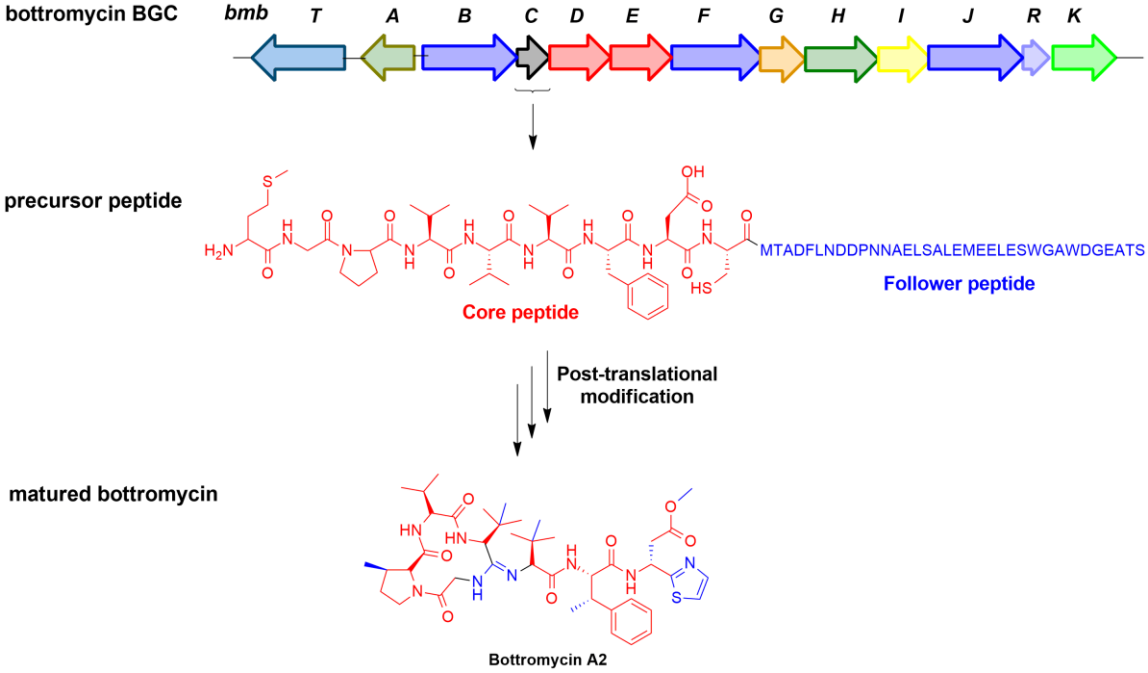
Abstract:
Bottromycin is a structurally complex cyclic peptidic compound isolated from *Streptomyces bottropensis* and related organisms and belongs to the RiPP natural products (ribosomally synthesized and post-translationally modified peptides). It exhibits potent antibacterial properties against gram-positive pathogens (including drug resistant strains such as *MRSA*, MIC 1 µg/mL and *VRE*, MIC 0.5 µg/mL) and mycoplasma. Bottromycin blocks the binding of the aminoacyl-tRNA to the A-site on the 50S ribosome and hence inhibits protein synthesis. Bottromycins contain structurally diverse post-translational modifications (PTMs) on a small peptide (GPVVVFDC) including a unique macrocyclic amidine, rare β-methylation, terminal thiazole heterocycle, oxidative decarboxylation, and Asp epimerization, among others. Unlike other RiPPs, it exhibits a unique precursor peptide structure with a C-terminal follower and a N-terminal core. This talk will highlight the current advancements in understanding the biosynthetic pathway of bottromycin focusing mainly on the biochemically and structurally characterized enzymes of the biosynthetic gene cluster (BGC) and intricate details of the peptide-protein interactions. These studies have provided a strong foundation for conducting combinatorial biosynthesis to create novel bottromycin variants for therapeutic applications.



References and Notes:

1. Schwalen, C.J.; Hudson, G.A.; Kosol, S.; **Mahanta, N.** et al *J. Am. Chem. Soc.*, **2017**, 139 (50), 18154-18157.
2. **Mahanta, N.**; Hudson, G.A. Mitchell, D.A. *Biochemistry* **2017**, 56 (40), 5229-5244.
3. Krushnamurthy, PH.; Subramanya, K.S.; Das, S.; Dhananjaya, G.; **Mahanta, N.*** *in review*, **2022**.
4. Krushnamurthy, P.H.; Kalakutagi, I.; **Mahanta, N.*** *manuscript in preparation*.

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

Nilkamal Mahanta
Designation: Assistant Professor and Head

Department of Chemistry
Indian Institute of Technology Dharwad
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I have received bachelor's degree in Chemistry from the University of Delhi (Hindu College) in 2005 and Master's in Chemistry from IIT Delhi in 2007. After a short stint of lectureship at Zakir Hussain College of Delhi University, I went to Texas A&M University, Texas, USA in 2009 to pursue higher studies. I worked on vitamin K biosynthesis and enzyme chemistry under the supervision of Prof. T. Begley which earned me a PhD degree in 2015. Thereafter, I joined Prof. Douglas Mitchell's lab at the Institute for Genomic Biology and Department of Chemistry at the University of Illinois, Urbana-Champaign, USA to conduct post-doctoral work on antibiotic ribosomal natural products and peptide/protein modifications. In Dec 2018, I joined the Department of Chemistry, IIT Dharwad as an assistant professor and currently serving as the Head of the department.

My research interests are in the field chemical biology, bioorganic chemistry, enzyme mechanisms, and antibiotic/anticancer natural products and presently guiding several PhD students. Notable recognitions in the academic career include Prof. M. K. Rastogi Award and Prof Seshadri Award (University of Delhi), Post-Graduate Merit Scholarship (UGC), Merit cum means scholarship (IIT Delhi), F. A. Cotton research award and Dow chemical research scholar award (Texas A&M University), C.S. Marvel postdoctoral award (University of Illinois, Urbana), ACS research award (American Chemical Society) and Acharya Prafulla Chandra Ray Award of Excellence (Indian Chemical Society, Kolkata).

Representative publications:

1. Andi Liu, P.H. Krushnamurthy, K.S. Subramanya, Douglas Mitchell, and **Nilkamal Mahanta***, *Methods in Enzymology*, **2021**, 656, 459-494 (*corresponding).
2. Andi Liu, Yuanyuan Si, Shi-Hui Dong, **Nilkamal Mahanta**, Haley N. Penkala, Satish K. Nair, and Douglas A. Mitchell., *Nature Chemical Biology*, **2021**, 17, 585-592.
3. Timothy W. Precord, **Nilkamal Mahanta**, and Douglas A. Mitchell, *ACS Chemical Biology*, **2019**, 14 (9), 1981-1989.
4. **Nilkamal Mahanta**, Katherine A. Hicks, Saad Naseem, Yang Zhang, Dmytro Fedoseyenko, Steven E. Ealick, and Tadhg P. Begley., *Biochemistry*, **2019**, 58 (14), 1837-1840.
5. **Nilkamal Mahanta**, Andi Liu, Shihui Dong, Satish K. Nair, and Douglas A. Mitchell. *Proceedings of the National Academy of Sciences, U.S.A.*, **2018**, 115 (12), 3030-3035.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Dr. Manisha Patni

Head & Associate Professor
Department of Chemistry
IIS (Deemed to be University)
SFS, Gurukul Marg, Mansarovar,
Jaipur-302020, Rajasthan
Contact Number: 9783307131
e-Mail: Manisha.patni@iisuniv.ac.in

Recent Picture

Manisha Patni graduated with M.Sc. Degree in Organic Chemistry and secured a Gold Medal from M. D. S. University, Ajmer. She obtained her Ph.D. in the Chemistry of Triazoles from University of Rajasthan in 2015. Her research interests include Synthetic Organic and Computational Chemistry with an emphasis on investigation of chemical reactivity, develop synthetic methods to augment the chemical toolbox, and collaborate to evaluate new therapeutic agents.

She has almost 25 years of teaching and 10 years of research experience and published papers in various journals of National and International repute. She has also presented papers in various National and International Conferences in India and Abroad. She acts as a catalyst to improve the quality of student learning in higher education by Research- Teaching integration. She is also a recipient of Certificate of Appreciation from All India Welfare Society for her contribution in the field of education.

Theoretical investigations of the microscopic mechanisms of heterogeneity and catalytic communication within single nanocatalysts

Srabanti Chaudhury*
Department of Chemistry
Indian Institute of Science Education and Research, Pune
(Email: srabanti@iiserpune.ac.in)

Abstract:

Nanoparticles are heterogeneous catalysts in terms of differences in size, shape, and surface sites leading to time dependent, particle-specific catalytic activity. The intrinsic heterogeneity of nanocatalysts complicates understanding the mechanisms of chemical processes in these systems using ensemble bulk measurements. Single molecule measurements showed strong temporal fluctuations in chemical reaction rates that depend on the size of the nanoparticles. Another important observation in nanocatalysts is the communication between different catalytic sites and such correlations extend over distances of few nanometres and persisting for hundreds of seconds. We developed a theoretical model to investigate the microscopic mechanisms of all these phenomena. This is based on a discrete-state stochastic description that allows us to explicitly evaluate dynamic properties of the system via stationary-state and first-passage probability density calculations. This description accounts for the stochasticity of individual chemical reactions at each catalytic site on a single NP and one can solve this model analytically for any number of active sites for all ranges of relevant parameters. Our theoretical investigation describes a possible microscopic origin of cooperative communications in nanocatalysts. The proposed theoretical framework quantitatively clarifies some important aspects of the microscopic mechanisms of heterogeneous catalysis.

References and Notes:

1. Chaudhury, S.*; Kolomeisky, A. B.*; *J. Phys. Chem. Lett.* **2020**, 11, 2330–2335
2. Punia, B.; Chaudhury, S.*; Kolomeisky, A. B.*; *J. Phys. Chem. Lett.* **2021**, 12, 11802–11810
3. Punia, B.; Chaudhury, S.*; Kolomeisky, A. B.*; *Proc. Natl. Acad. Sci. U.S.A.* **2022**, 119, e2115135119

Bio-Sketch of the Speaker

Dr. Srabanti Chaudhury

Associate Professor

Department of Chemistry,
IISER Pune

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Email: srabanti@iiserpune.ac.in

Home Page: https://sites.google.com/site/srabantic01/

Dr. Srabanti Chaudhury did her PhD in Theoretical Chemistry from IISc Bangalore under the supervision of Prof. Binny Cherayil in 2009. She joined as a postdoctoral fellow at Rice University followed by University of Texas at Austin and at Los Alamos National Laboratory. She started her independent career as an Assistant Professor at IISER Pune in the department of Chemistry in 2013. Currently she is an Associate Professor at IISER Pune and also the Associate Dean of Doctoral Studies at IISER Pune. She is the Associate Editor of the journal Frontiers Biophysics. Her research interests involve development of theoretical models to investigate stochastic fluctuations in chemical physics, biology and soft condensed matter using the concepts of statistical mechanics.

Awards/ Recognitions:

Dr. Chaudhury received the bronze medal awarded by Chemical Research Society of India(CRSI) in 2022. She was selected for the Japan-Asia Youth Exchange Program in Science (Sakura Exchange Program in Science 2018) administered by Japan Science and Technology Agency.

Representative publications:

Biophysical J. **2022**, 121, 2398–2410
Proc. Natl. Acad. Sci. U.S.A. **2022**, 119, e2115135119
J. Phys. Chem. B **2021**, 125, 4536–4545
J. Phys. Chem. Lett. **2020**, 11, 2330–2335
J. Phys. Chem. B, **2018**, 122, 360–368
J. Chem. Phys. **2017**, 146, 145103
J. Phys. Chem. B **2014**, 118, 10405 -10412

Magnetic Fields in Chemistry - Semiconductors to Stars

Sangita Sen*
Department of Chemical Science
Indian Institute of Science Education and Research
(Email: sangita.sen@iiserkol.ac.in)

Abstract:

Looking at stars through the window has stirred many a scientific mind but to find out what they are made of only by looking at them needs us to harness our knowledge from several fields including chemistry. In this presentation I wish to discuss the role of quantum chemistry in astrophysics in the context of magnetic stellar objects. I will also discuss how methodologies developed to aid in the exploration of stars can potentially be validated by experiments on semiconductors.

Bio-Sketch of Speaker

Sangita Sen
Assistant Professor

Department of Chemical Sciences
Indian Institute of Science Education and Research

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PhD in Chemistry - Indian Association for the Cultivation of Science, Kolkata
Marie-Curie Individual Fellowship for Post-doctoral work

Selected Publications:

1. "*Excited States of Molecules in Strong Magnetic Fields"*
S. Sen, K.K. Lange and E.I. Tellgren, J. Chem. Theory Comput. 15, 3974 (2019)

2. "*Non-perturbative calculation of orbital and spin effects in molecules subject to non-uniform magnetic fields"*
S. Sen and E.I. Tellgren, J. Chem. Phys., 148, 184112 (2018) : Editor's Pick

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
…Anticipating Tomorrow's Science through Collaborative Ventures

Joyanta Choudhury

Professor

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IISER Bhopal

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In 2006, Joyanta Choudhury received his PhD degree from IIT Kharagpur, India. After two postdoctoral stints at The Scripps Research Institute in Florida with Prof. Roy A. Periana and at the Weizmann Institute of Science with Prof. Milko E. van der Boom as a Marie Curie International Incoming Fellow, he joined the Department of Chemistry, IISER Bhopal, India, in 2011, where he is currently working as a Professor.

His research group is involved in pioneering the area of '*transition metal-NHC platform-based annulative π-extension chemistry*'. In parallel, his group has conceptualized the development of '*stimuli switchable metal-NHC catalysts*' for reversible chemical H_2 storage-delivery applications in the form of liquid hydrogen carriers (LHC) (viz. *N*-heterocycles/hydrogenated *N*-heterocycles, and CO_2/HCOOH couples) as potential alternative and clean energy vectors. He was awarded with the CRSI Bronze Medal in 2019. He serves as an Editorial Advisory Board Member in *ACS Catalysis* and *Tetrahedron Green Chemistry*.

Representative Publications:

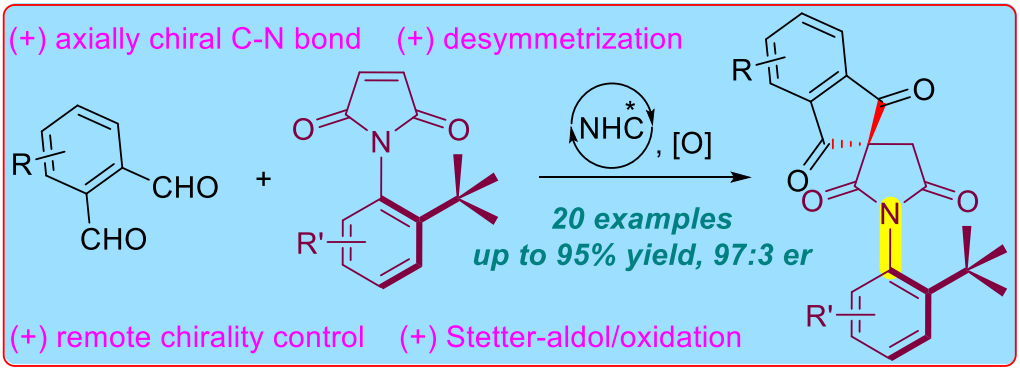
1. Transfer Hydrogenation of CO_2 and CO_2-Derivatives using Alcohols as Hydride Sources: Boosting an H_2–Free Alternative Strategy. *ACS Catal.* **2022**, *12*, 8886–8903 (*Perspective*).
2. Cationic π-Extended Heteroaromatics via Catalytic C–H Activation Annulative Alkyne-Insertion Sequence. *Chem. Commun.* **2022**, *58*, 133-154 (*Feature Article*).
3. Emerging Implications of the Concept of Hydricity in Energy-Relevant Catalytic Processes. *Chem. Eur. J.* **2021**, *27*, 5842 –5857 (*Minireview*).

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

N-Heterocyclic Carbene (NHC)-Catalyzed Synthesis of C-N and N-N Axially Chiral Molecules

Akkattu T. Biju*
Department of Organic Chemistry, Indian Institute of Science, Bangalore-560012, India
(Email: atbiju@iisc.ac.in)

Abstract: N-Heterocyclic carbene (NHC)-catalyzed umpolung of aldehydes is widely used for the unconventional access to target molecules.[1] Although the assembly of axially chiral C-C bonds leading to the atroposelective synthesis of biaryls and related compounds are well-known, the analogous synthesis of compounds bearing axially chiral C-N bonds are relatively rare. We have recently reported the NHC-catalyzed atroposelective synthesis of N-aryl succinimides having an axially chiral C-N bond via the desymmetrization of N-aryl maleimides.[2] The NHC involved intermolecular Stetter-aldol cascade of dialdehydes with prochiral N-aryl maleimides followed by oxidation afforded N-aryl succinimides in good yields and ee values. Preliminary studies on rotation barrier for the C-N bond, the temperature dependence, and detailed mechanistic studies are also being presented. Moreover, very recent studies on kinetic resolution of amino substituted N-aryl maleimides will be presented.[3] Furthermore, NHC-catalyzed route for the synthesis of compounds containing axially chiral N-N bond also will be discussed.[4]



References and Notes:

1. For reviews, see: (a) Flanigan, D. M.; Romanov-Michailidis, F.; White, N. A. Rovis, T. *Chem. Rev.* **2015**, *115*, 9307. (b) Enders, D.; Niemeier, O.; Henseler, A. *Chem. Rev.* **2007**, *107*, 5606. For a Book, see: (c) Biju, A. T. *N-Heterocyclic Carbenes in Organocatalysis*; Wiley-VCH Verlag GmbH & Co. KGa A: Boschstr. 12, 69469 Weinheim, Germany, 2019.
2. Barik, S.; Shee, S.; Das, S.; Gonnade, R. G.; Jindal, G.; Mukherjee, S.; Biju, A. T. *Angew. Chem. Int. Ed.* **2021**, *60*, 12264.
3. Barik, S.; Das, R. C.; Balanna, K.; Biju, A. T. *Org. Lett. (Under revision).*
4. Balanna, K.; Shee, S.; Barik, S.; Barik, S.; Biju, A. T. *(Manuscript Submitted).*

Bio-Sketch of Speaker

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Editor, *J. Heterocyclic Chem*.
Advisory Board, *Org. Chem. Front*.
International Advisory Board, *Asian J. Org. Chem*.
Editorial Board, *Green Synth. Catal*.

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

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Sensitive free cysteine detection and rapid protein bioconjugation via facile Michael addition-elimination reactions

Dimpy Kalia*
Department of Chemistry
Indian Institute of Science Education and Research (IISER) Bhopal, India
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Abstract:

In my talk, I will discuss our recent work on the development of two facile Michael addition-elimination reactions, and their use for the sensitive detection of free Cys (an established oxidative stress biomarker) and for rapid protein bioconjugation. One of these reactions enabled the development of Michael addition-elimination-cyclization turn-on fluorescence (MADELCY TOF) probes that selectively react with free Cys over other biothiols such as homocysteine and glutathione. Our most sensitive MADELCY TOF probe demonstrated a detection limit of 8.2 nM for free Cys and a fluorophore release $t_{1/2}$ of <3 min, enabling the sensitive detection of free Cys in blood plasma. This probe also enabled the sensitive estimation (detection limit = 9.5 pM) of the cancer and liver cirrhosis biomarker enzyme, aminoacylase-1 (ACY-1). Another probe of this series enabled the live cell imaging of free Cys, allowing us to monitor H_2O_2-induced oxidative stress in mammalian cells. The second Michel addition-elimination reaction that we have developed enabled the selective labeling of *N*-terminal Cys residues of proteins. Notably, this method is diastereoselective, proceeds in quantitative yields, and demonstrates remarkably rapid reaction kinetics (k_2 = 3×10^3 $M^{-1}s^{-1}$) at stoichiometric low micromolar amounts of bioconjugation reagents under physiological conditions. These results underline the tremendous scope of 1,2-aminothiol-triggered cascaded reactions of Cys for diverse applications.

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

Dr. Dimpy Kalia
Assistant Professor
Department of Chemistry
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Homepage: https://sites.google.com/iiserb.ac.in/dimpy-lab/

Dimpy obtained her B.Sc. degree from Government College for Girls, Chandigarh and her M.Sc. (Honours) in Organic Chemistry from Panjab University, Chandigarh. Thereafter, she worked in a pharmaceutical company (Aurigene Discoveries Technology Ltd., Bangalore) for a year before joining Dr. Dinesh K. Dikshit's laboratory at the Central Drug Research Institute (CDRI), Lucknow as a Ph.D. student. Her Ph.D. research focused on the synthesis of small natural products and on the medicinal chemistry of *M. tuberculosis*. After completing her Ph.D. in 2010, Dimpy started her second stint at Aurigene (Bangalore) where her work focused on the synthesis of several complex small molecules. In 2012, Dimpy joined Prof. Herman O. Sintim's research group at the University of Maryland, College Park, U.S.A. as a postdoctoral researcher, where her work focused on a wide range of topics at the interface of chemistry and biology including the development of selective ligands for G-quadruplexes and bacterial signaling mediated by the second messenger, c-di-GMP. After her postdoctoral tenure, Dimpy worked as IISER Fellow at IISER Pune and then moved to the University of Pune in January 2014 as a DST-INSPIRE Faculty to set up her independent research group. She joined IISER Bhopal in January 2018 as an Assistant Professor. Research in Dimpy's laboratory lies at the chemistry-biology interface and focuses on organic synthesis and on developing chemical-biology based methods for addressing questions of biological importance. The current research areas of the lab are: developing facile approaches for protein bioconjugation, chemical biology of c-di-GMP signaling in bacteria, and developing new concise methods for the synthesis of complex heterocyclic small molecules.

Career Profile:

S No	Positions held	Name of the Institute	From-To
1	Research Associate (Industry)	Aurigene Discoveries Technologies Ltd.	July 2004- Apr 2005
2.	Ph.D. student	CDRI Lucknow	May 2005- Dec 2010
2	Junior Scientist (Industry)	Aurigene Discoveries Technologies Ltd.	Jan 2011-Mar 2012
3	Postdoctoral Fellow	University of Maryland, College Park, USA	Mar 2012-Apr 2013
4	IISER Fellow	IISER Pune	July 2013- Dec 2013
5	DST-INSPIRE Faculty	Department of Chemistry, University of Pune (now known as Savitribai Phule Pune University)	Jan 2014-Jan 2018
6	Assistant Professor	Department of Chemistry, Indian Institute of Science Education and Research (IISER) Bhopal	Jan 2018- present

Significant awards/achievements:

S No	Name of the Recognition/Award / Fellowship	Awarding Agency
1	Awarded SERB-POWER grant (Apr 2022-Apr 2025)	SERB
3	Invited to serve as a member of the International Advisory Board of the European Journal of Organic Chemistry (Jan 2021-present)	Wiley-VCH
6	Awarded the Early Career Research Award (ECRA) by SERB, India (Mar 2019-Mar 2022).	SERB
14	DST-INSPIRE Faculty Award (Jan 2014-Dec 2018)	DST

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Deepak Chopra

Professor

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Homepage: https://chm.iiserb.ac.in/faculty_profile.php?id=Mg==&lname=ZGNob3ByYQ==

Career Profile
Assistant Professor: IISER Bhopal, 2009 – 2015.
Associate Professor: IISER Bhopal, 2015 – 2021.
Professor: Since 2021

Significant Awards/ Achievements
1. **University Gold Medal** on being ranked **1st** in the **Department of Chemistry**, **Jadavpur University** in **BSc** (**Chemistry Honours**).
2. **Bruker AXS India- Best Poster Award** for the **Best Poster Prize** at the **36th National Seminar in Crystallography** at **University of Madras**, held from **January 20-24, 2007**.
3. Member of the Editorial Board of **"Journal of Molecular Structure". The link is http://www.journals.elsevier.com/journal-of-molecular-structure/editorial-board**
4. **Co-Editor** of **Acta Crystallographica E**, IUCr publications since August 2017.
5. Selected as a **Sakura Science Fellow**, **2018** to visit **Osaka University, Japan** (November 24 – December 1 2018).
6. Elected as "**Fellow of Indian Chemical Society**" in **2019**.
7. Elected as "**Fellow of Royal Society of Chemistry (FRSC)**, in November 2020.
8. Recognized by the Editors of the RSC Journal, **CrystEngComm** as an "**Outstanding Reviewer**" for the year **2020**.
9. Nominated to the **Advisory Board** of the **RSC journal**, **CrystEngComm** for a period of two years (**2021 -2023**).

Representative Publications:

1. ***Cryst. Growth Des***., 2014, 14, 3155-3168.
2. ***CrystEngComm.,*** (Cover Page), 2015, 17, 3596–3609
3. ***Chem Commun.***, 2016, 52, 2141-2144.
4. ***Chem Commun.***, 2016, 52, 7225 – 7228.
5. ***Phys.Chem.Chem.Phys.***, 2016, 18, 13820-13829.
6. ***Chem. Eur. J.***, (Communication), 2017, 23, 1023-1027.
7. ***J. Phys. Chem. C*** (Cover Page). 2019, 123, 9311-9322.
8. ***ChemComm.***, 2020, 56, 12841-12844.
9. ***J. Am. Chem. Soc.,*** 2021, 143, 1024−1037.
10. ***J. Mater. Chem. C.,*** 2022, 10, 4257 - 4267.

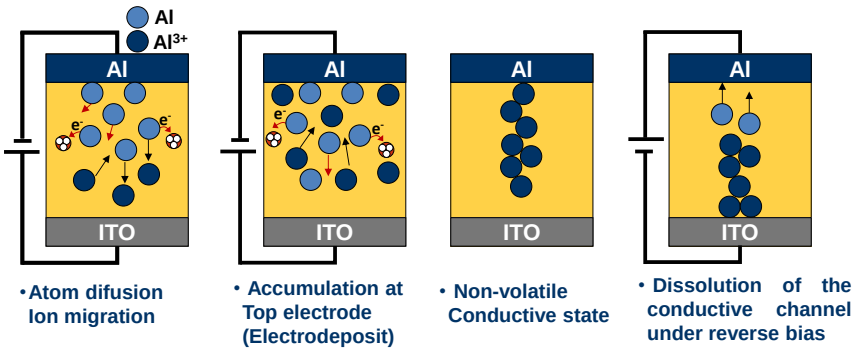
Benignant Electron Carrier Traps in Organic Semiconductors for Electrical Bistability

Ratheesh K. Vijayaraghavan

Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata (IISER- K), West Bengal, Indi)
Email: ratheesh@iiserkol.ac.in

Abstract:
Charge carrier traps (**CCT**) are considered to be highly detrimental for the performance of most of the organic semiconductor (OSC) devices such as Organic Field Effect Transistors (**OFETs**), Organic Solar Cells (**OSC**) comprising OSC active layer (**AL**) processed under ambient environmental conditions. The present poster will describe our attempt of the functional utilization of this highly derogatory attribute (CCT) of tailored organic semiconductors to yield high performance organic memristor devices. The idea of translating the bulk charge traps as the cause to nucleate switchable electrical bistability (bistable conducting states) in metal-semiconductor metal (MSM) sandwich devices. Switching between two conducting state is the primary requisite of memristors or resistive memory devices that are considered as an essential electrical component in data processing and information technology. The bistable and switchable conductive states (ON & OFF or '0' & '1') can be assigned as the binary data storage and if it is reversible, it could be rewritable as well. Having a non-volatile nature to the stored data would make such devices superior over the volatile one with respect to the wide range of use. Here, we demonstrate the switching mechanism bases on the initial results of trap assisted control on the resistive state switching in Metal-Semiconductor-Metal devices with a precise control over the trap density by carefully designed chemical structures resulted in regulating the formation of conductive filaments persuaded in tuning the ON/OFF current ratio in resistive memory devices.

Figure/Scheme (if any):



Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

Dr. Rathesh K. Vijayaraghavan
Associate Professor

Department of Chemical Sciences
IISER Kolkata

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4. Academic Qualification (Undergraduate Onwards)

	Degree	Year	Subject	University /Institution
1	B.Sc.	2002	Polymer Chemistry	University of Calicut
2	M.Sc.	2004	Applied Chemistry	University of Calicut
3	Ph. D	2011	Chemistry	National Institute for Interdisciplinary Science and Technology(CSIR)/ University of Kerala

5. Ph.D thesis title, Guide's Name, Institute/Organization/University, Year of Award:

Title: Design, synthesis and study of photoresponsive liquid crystals and investigation of light emitting properties of their solid and liquid crystalline phases.

Guide's Name: Dr. Suresh Das

Institute: Photosciences and Photonics Group, National Institute for Interdisciplinary Science and Technology (NIIST, CSIR), Trivandrum, India.

Year of award: 2011

6. Work experience (in chronological order).

	Position Held	Name of the Institute	From	To
1	Postdoctoral Fellow	Molecular Materials and Nanosystems, Technical University of Eindhoven	April 2011	
2	Asst. Professor (On Contract)	IISER Kolkata	July 2015	January 2016
3	Asst. Professor	IISER Kolkata	February 2016	June 2021
4	Assoc. Professor	IISER Kolkata	June 2021	Till date

Self-Templated Conversion of A Self-healing Metallogel into Active Photocatalyst for CO_2 Reduction

Noohul Alam and Debajit Sarma*
Department of Chemistry
Indian Institute of Technology Patna
(Email: debajit@iitp.ac.in)

Abstract:

Light-assisted conversion of CO_2 into fuels and feedstocks in presence of water mimics the natural photosynthesis process. This is a clean and sustainable technique to alleviate the energy shortage, as well as global climate change. In this context, herein, a new waterborne self-healing metallogel (Nd-SHMG) along with a self-templated carbonization strategy is presented for the synthesis of neodymium@nitrogen-doped carbon quasiaerogel (Nd@NCA) catalyst. A metal-free nitrogen-doped carbon quasiaerogel (MF@NCA) was also prepared *via* the selective removal of the metal from Nd@NCA catalyst. The as-synthesized Nd@NCA and MF@NCA catalysts are composed of highly porous 2D-sheets which are grown on top of each other adopting the 3D foam-type structure. The selective removal of the metal results in a 9 fold increase in the BET-specific surface area and a 30-fold increase in the CO_2 adsorption capacity of the MF@NCA catalyst over the pristine Nd@NCA catalyst. The as-synthesized Nd@NCA photocatalyst shows excellent activity with high selectivity (87%) for CO_2 conversion into CO as compared to CH_4 and H_2 (Figure 1).

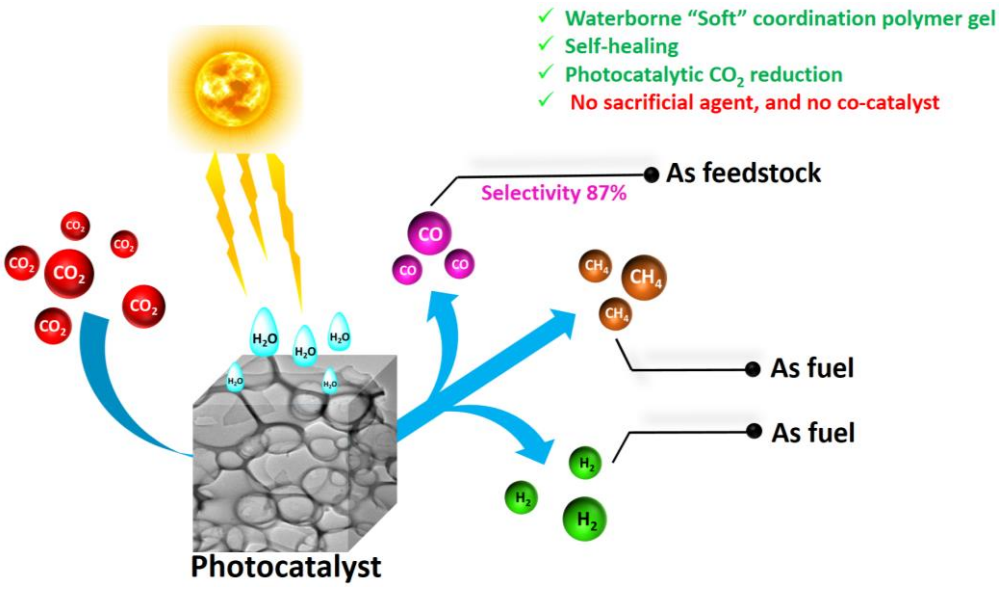

Figure 1. Image illustrating the photocatalytic CO_2 reduction by water in the presence of light.

References and Notes:

1. Alam, Noohul.; Sarma, Debajit. (Unpublished Work).

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

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Debajit Sarma is an Assistant Professor in the Department of Chemistry, Indian Institute of Technology Patna, India. He received his PhD from Indian Institute of Science, Bangalore (IISc), in 2012. He had a postdoctoral stint at Northwestern University, Evanston, USA from 2013 to 2016 in the group of Prof. Mercouri G. Kanatzidis.

His broad area of research is inorganic and solid-state materials within the framework of coordination polymer, oxides and metal chalcogenides. Such material ranges from discrete molecular compounds, coordination polymer to solid state inorganic materials. These materials are expected to contribute to the current technology in electronics, energy, and environment. The objective is to pursue deeper understanding and hence control over the synthesis-structure-function correlation to bond fundamental research with technology.

He is a recipient of Science & Engineering Research Board (SERB) Early Career Research Award. He has published more than 35 papers in repute international journal along with 2 US patents.

Representative publications:

1. Thakre, Dewendra; Ali Sk Rajab; Mehta, Sakshi; Alam, Noohul; Ibrahim, Masooma; **Sarma, Debajit**; Mondal, Abhishake; De, Mrinmoy; Banerjee Abhishek. *Cryst. Growth Des.* **2021**, *21*, 4285−4298.
2. Alam, Noohul; **Sarma, Debajit**. *Soft Matter*, **2020**,*16*, 10620-10627.
3. Alam, Noohul; **Sarma, Debajit**. *ACS omega*, **2020**, *5*, 17356-17366.
4. Kuilya, Hemrupa; Alam, Noohul; **Sarma, Debajit**; Choudhury, Diganta; Kalita, Apurba. *Chem. Commun*. **2019**, *55*, 5483-5486.
5. Feng, Mei-Ling; **Sarma, Debajit**; Gao, Yu-Jie; Qi, Xing-Hui; Li, Wei-An; Huang, Xiao-Ying; Kanatzidis, Mercouri G. *J. Am. Chem. Soc.* **2018**, *140*, 11133–11140.
6. Rapti, Sofia; Sarma, Debajit; Diamantis, Stavros A.; Skliri, Euaggelia; Armatas, Gerasimos S.; Tsipis, Athanassios C.; Hassan, Youssef S.; Alkordi, Mohamed; Malliakas, Christos D.; Kanatzidis, Mercouri G.; Lazarides, Theodore; Plakatouras, John C.; Manos, Manolis J. *J. Mater. Chem. A* **2017**, *5*, 14707-14719.
7. **Sarma, Debajit**; Malliakas, Christos D.; Subrahmanyam, K. S.; Islam, Saiful M.; Kanatzidis, Mercouri G. *Chem. Sci.* **2016**, *7*, 1121-1132.

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Mohammad Qureshi is currently a full Professor of department of chemistry at Indian Institute of Technology Guwahati. He received his Ph.D. in chemistry from Indian Institute of Technology Kanpur on organic light emitting diodes. After a brief stint at National Taiwan university, he moved to Forschungzentrum Juelich, Germany for his postdoctoral studies as a Helmholtz Fellow.

In 2008, he started his independent research career as an Assistant Professor at IIT Guwahati. His research focuses on photo(electro)catalytic conversion of water into hydrogen and oxygen, quantum dot and dye sensitized solar cells and sensors for medical diagnostic applications. He has been invited to be the fellow of royal society of chemistry (FRSC), London in 2021. He is receipt of Sakura Science Award (2019) and Fulbright – Nehru Academic and Professional Excellence fellowship (2017).

Elucidating ultrafast excited-state dynamics of *mKeima*: Hidden conformers and stepwise versus concerted isomerization and proton transfer

Garima Bhutani[$], Pratima Verma[#], Kausik Chattopadhyay[#] and Arijit K. De[$]*
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Abstract:

Green fluorescent protein (GFP) of the jellyfish *Aequorea Victoria* was discovered by Osamu Shimomura in the early 1960s and the widespread interest in exploring with GFP arises mainly due to the chromophore formation (4-(p-hydroxybenzylidene) imidazolinone) by the autocatalytic, post-translational modification involving cyclization and oxidation of three consecutive amino acids at position 65-67, such as Ser, Tyr, and Gly which is responsible for their fluorescence. Subsequently, various fluorescent proteins (FPs) with yellow, orange and red fluorescence were engineered through mutagenesis in GFP, resulting in modification of chromophore structure and the protein environment. Furthermore, different colored FPs were identified from non-bioluminescent Anthozoa homologs of GFP. Among several FPs, red fluorescent proteins (RFPs) gained attention for their large "pseudo-Stokes shift" with for applications in deep-tissue and whole-body imaging because of low light scattering, reduced auto-fluorescence etc. The chromophore of red fluorescent proteins (RFPs) has an extended N-acylimine group comparative to GFP chromophore which principally increases the conjugation and thus fluoresces in higher wavelength regions. Two ground state forms of *wt*-GFP and *mKeima* (variant of RFP) have been known: neutral form & anionic form. The neutral form after excitation, undergoes an excited-state proton transfer (ESPT) on a timescale of a few picoseconds, yielding the anionic form in the excited state which then fluoresces, and finally returns to neutral form via proton back-transfer in the ground state, termed as ground state proton transfer (GSPT). Moreover, unlike GFP, *mKeima* chromophore exists predominantly in anionic/neutral form in acidic/basic environment which is known as "*reverse protonation effect*".

In this work, we have investigated the conformational heterogeneity of the neutral and anionic form of chromophore in different pH environment. In addition, the role of the local environment of protein on the ultrafast excited-state dynamics (i.e., ESPT) coupled with the conformational changes of chromophore following reverse protonation is explored. We further investigated the origin of dual-fluorescence in *mKeima* at low pH conditions and compared the competitive pathways of dual-fluorescence versus ESPT at extreme pH conditions.

Abstract - Invited Lecture

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Bio-Sketch of Speaker

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Arijit Kumar De was born in Kolkata (formerly Calcutta in WB, India) and was raised in the suburbs where he had his schooling. He completed his BSc (2003) with a major in Chemistry from the Ramakrishna Mission Residential College, Narendrapur (affiliated to the University of Calcutta, WB, India) and MSc (2005) in Chemistry from IIT Kanpur (UP, India). He pursued his PhD with Prof Debabrata Goswami at IIT Kanpur (2005-2010) working on two-photon fluorescence microscopy and optical trapping. He was a postdoctoral fellow at the Lawrence Berkeley National Lab and the University of California Berkeley (CA, USA) with Graham R. Fleming (2010-2014) where he developed two-dimensional fluorescence-detected coherent spectroscopy (2D-FDCS). In 2014, he joined IISER Mohali (PB, India) where he is now an Associate Professor in the Department of Chemical Sciences.

The central theme of research in the "Condensed Phase Dynamics" group at IISER Mohali led by him is to explore, through a combination of theory and experiments, a wide range of problems in chemistry, biophysics, and condensed matter physics. For this, the group has developed some cutting-edge spectroscopic techniques (for example, sub-20 fs broadband pump-probe spectroscopy, two-dimensional electronic spectroscopy, pump-dump-probe spectroscopy, time-resolved impulsive stimulated Raman spectroscopy, multimodal optical tweezers, holographic beam shaping, etc.). More specifically, the main focus of the group is to investigate energy and charge (electron or proton) transfer dynamics, covering a wide range of time scales (few tens of femtoseconds to few tens of nanoseconds), within a variety of systems (molecular aggregates, photovoltaic systems, fluorescent proteins, etc.) and the effect of local environment (for example, solvation, nanoscale confinement, etc.) on it. The group also pioneered deciphering the role of optical and thermal nonlinearities in laser trapping under femtosecond pulsed excitation.

Functional Dye-TEG Amphiphiles for Self-cleaning, Self-sterilizing fabric and Bio-imaging Applications

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Abstract: Introducing a unique and smart functionality in a dye, in addition to the coloring property, which is the original performance of a dye has widened the horizon for functional dye applications. Our research group has been successful in developing a self-sterilizing and self-cleaning fabric by the simple application of a dye; and a bio-imaging agent that may destroy cancer cells categorically prohibiting cancer cell migration specifically designed for skin application. We have tailored two designer dyes having absorption in two different regions of the visible light spectrum and conjugated with tetraethylene glycol (TEG) for improved hydrophilicity, biocompatibility, and inhibition of immunogenicity. A NIR class dye, Metallo-phthalocyanine ($ZnPc(TEG)_4$) consisting of four tetraethylene glycols covalently attached to four peripheral positions has been synthesized. The resultant amphiphilic $ZnPc(TEG)_4$ dye is soluble in both organic solvent and aqueous medium; exhibits high singlet oxygen quantum yield ($\phi_\Delta = 0.8$) leading to an excellent photo-sensitizer (Fig. 1). In addition, benzothiazole class of dye, a neutral Thioflavin-T [2-(4´,4´-dimethylaminophenyl)benzothiazole, BTA-2] covalently attached to the tetraethylene glycol (TEG-BTA-2) was synthesized. Conjugation of a TEG molecule enables the neutral TEG-BTA-2 amphiphile to exhibit aggregation-induced emission (AIE) in the water-THF system making a potential neutral amphiphilic dye candidate for bioimaging application (Fig.2). Synthesis, photophysical properties of both the dyes $ZnPc(TEG)_4$ and TEG-BTA-2, detailed investigation on photo-dynamic property of $ZnPc(TEG)_4$ for self-sterilizing and self-cleaning applications, AIE behaviour of TEG-BTA-2 and bioimaging application will be presented.

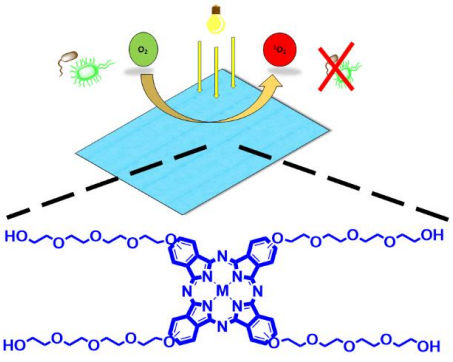

Figure. 1. $MPc(TEG)_4$ photosensitizer dyed self-sterilizing and self-cleaning cotton fabric.

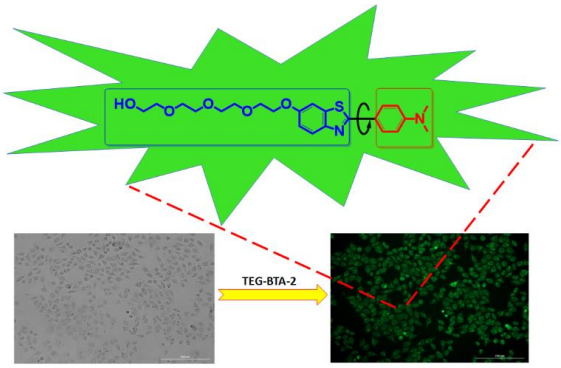

Figure. 2. TEG-BTA-2 conjugate amphiphile as a bioimaging agent for cancer cell.

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1. Verhoef, J. J. F.; Anchordoquy, T. J.; *Drug Deliv. Transl. Res.* **2013**, *3*, 499–503.
2. Lo, P. C.; Rodríguez-Morgade, M. S.; Pandey, R. K.; Ng, D. K. P.; Torres, T.; Dumoulin, F. *Chem. Soc. Rev.* **2020**, *49*, 1041–1056.
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4. Qin, L.; Vastl, J.; Gao, J. *Mol. Biosyst.* **2010**, *6*, 1791–1795.

Bio-Sketch of Speaker

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Dr. Nabanita Sadhukhan received her M.Sc. from the University of Kalyani in 2002 and her Ph.D. from the Indian Institute of Technology Kanpur in 2009. After completing postdoctoral research at Tohoku University, Japan, she briefly worked at Central Leather Research Institute, Chennai (2014 – 2016). She has been presently working at ICT Mumbai as a UGC assistant professor since 2016. Her current research interests are

- Nature-inspired dye-based molecular glue for tumor and anti-cancer application.
- Synthesis of non-toxic trace element complexes for food, fodder and fertilizer application.
- Synthesis of tailored design functional dyes for self-cleaning and self-sterilizing textile material.
- Controlled release perfume encapsulated microcapsules for sanitary pad application.

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Dr. Ekambaram Balaraman received his M.Sc in Chemistry from R.K.M. Vivekananda College, Chennai (2002), and Ph.D from the Central University of Hyderabad (2008). Subsequently, he has been an FGS-Post Doctoral Fellow at the Weizmann Institute of Science (2008-2012). In July 2013, he started his independent career as a senior scientist at the CSIR-National Chemical Laboratory. In Dec'2018, he moved to the IISER-Tirupati as a faculty in chemistry. He is the recipient of the MRSI Medal (2021), SwarnaJayanti Fellowship (2020), CRSI-Bronze Medal (2020), The Asian and Oceanian Photochemistry Association (APA) for Young Scientist (2019), Fellow of Royal Society of Chemistry (2019), AV Rama Rao (AVRA) Young Scientist Award (2018). He is a member of the Indian National Young Academy of Science (INYAS), INSA (2018).

Dr. Balaraman's research primarily focuses on generating resources for green energy and recycling atmospheric waste. Specifically, he works on the design and development of catalytic materials for hydrogen generation from feedstocks, sustainable chemical synthesis, and conversion of CO_2 to value-added products. He is also interested in the development of electron donors for heterogeneous Ziegler catalysts used in the manufacture of isotactic polypropylene.

Selected Publications:

1. M. Subaramanian, M.; G. Sivakumar, **E. Balaraman***. First-row transition-metal catalyzed acceptorless dehydrogenation and related reactions: A personal account. *Chem. Rec*. **2021**, *21*, 3839–3871.
2. V. Yadav, V. G. Landge, M. Subaramanian, **E. Balaraman***. Manganese catalyzed α-olefination of nitriles with secondary alcohols. *ACS Catal*. **2020**, *10*, 947–954.
3. M. Subaramanian, S. P. Midya, P. M. Ramar, **E. Balaraman***. General synthesis of *N*-alkylation of amines with secondary alcohols via hydrogen autotransfer. *Org. Lett*. **2019**, *21*, 8899–890.
4. G. Jaiswal, V. Landge, D. Jagadeesan*, **E. Balaraman***, Iron-based nanocatalyst for the acceptorless dehydrogenation reactions, *Nature Commun*. **2017**, *8*, 2147–2160.
5. S. P. Midya, M. K. Sahoo, V. G. Landge, P. R. Rajamohanan and **E. Balaraman***. Reversed reactivity of anilines with alkynes in the rhodium-catalysed C–H activation/carbonylation tandem. *Nature Commun*. **2015**, *6*, 8591–8601.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
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Bio-Sketch of Speaker

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2016 – 2019, Managing Editor, American Chemical Society
2019 – 2021, *Associate Director*
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Royal Society of Chemistry Cambridge: Bangalore, Karnataka, IN
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2013-06 to 2014-11 | Postdoc Fellow (Chemistry)
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Recent Picture

Career Profile, significant awards/achievements: Alumni of IIM Ahmedabad, RDVV University, and Harvard Business School, Ajit is an experienced leader leading strategic and expansion initiative, a leading voice of diversity and inclusion and advocate for sustainability with over 23 years of experience in business management. Ajit has worked in STEM Education & research, Pharma, Healthcare and Analytical Chemistry areas in MNCs across APAC and European regions.

He feels privileged to have got the opportunity to facilitate the UK-India Innovation and Sustainability Consortium in 2021 where we managed to receive a grant from the UK government. He also conducted the RSE- Industry-Academia dialogue aimed to strengthen industry-academia collaborations and establish a robust innovation ecosystem in India. The objective of these collaborations is to drive research outputs toward sustainability, newer energy sources and gender diversity in research. We also help promote the cause of Open Science and Open Access. Besides, He has been working on various projects to promote gender diversity and working on community development.

Currently, he is working on advancing and developing the chemical sciences community in India and South Asia. Besides, He is collaborating with leading Indian academic institutes to develop educational and research programs with a mission to impact as many students from schools, colleges and universities.

He strongly believes that an inclusive and diverse workplace is crucial to a successful business. However, representing each group and making it possible for every employee equally involved goes far beyond policies and programs. It takes the proper implementation of diversity strategies.

The New Initiatives by Wiley in Recent Past

Khushbu Kushwaha*
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Abstract:
John Wiley & Sons, Inc., an American multinational publishing company founded in 1807, has become a global leader in publishing, education and research. In 2018, Wiley expanded its research publishing team with two new peer review handling editors in Chemistry based out of India. The idea was to publish more Indian content and involve more Indian researchers in the Editorial Boards of Wiley Chemistry journals. Altogether there are about ca. 25 Editorial Advisory Board Members from India over the twenty journals in the group. Wiley also has a strong connection with CRSI (Chemical Research Society of India) which is a part of ACES (Asian Chemical Editorial Society), a society-partner of Wiley. CRSI and ACES had taken part in many collaborative projects. For example, 1st ACES-CRSI symposium was organized in 2020.

Wiley is also committed to celebrate women in science and has taken several initiatives to empower women scientists in India and all-around world. Since its inception in 2019, Wiley has taken part in the IUPAC Women's Global breakfast event. Another way we support women in science is by publishing special issues highlighting and recognizing the efforts by women scientists from all around the world. We have been doing this on a regular basis since 2011, the International Year of Chemistry, the focus of which was the role of women in chemistry. We are also striving to increase diversity in our Editorial and Advisory boards.

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Khushbu Kushwaha obtained her PhD in Medicinal Chemistry from University of Delhi (India) in 2012. The topic of her research was synthesis of azaphenothiazine derived pharmacophores and their anticancer activity. She then relocated to Belgium and joined the organic synthesis group at University of Antwerp (UA) as postdoctoral research associate. At UA her work mainly focused on developing alternative and convenient methodologies for the synthesis of small and medium sized nitrogen heterocycles. Further, she spent two years at Department of Chemistry and Molecular Biology of GU as a Visiting Researcher and worked on developing liquid chromophores.

Overall, she published 20 research papers in high impact journals including, *Advanced Science*, *Science Advances*, *Advanced Synthesis and Catalysis*, *EJOC*, *The Journal of Physical Chemistry C*, *RSC Advances*, *BMCL*, *Physical Chemistry Chemical Physics* etc. She joined *ChemistrySelect* team of Wiley-VCH in August 2019 as an Associate Editor and based in Delhi (India). In 2021, she joined the team of *European Journal of Organic Chemistry* as an Associate Editor and *The Chemical Record* journal as Associate Managing Editor. She represents the whole porfolio of *Chemistry Europe* and *ACES* journals as an acquisition editor at conferences and workshops.

Bio-Sketch of Chairperson
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Dr Aparna Ganguly completed her graduation and post- graduation in Chemistry from University of Delhi and subsequently obtained her PhD in Materials Chemistry under the supervision of Professor A. K. Ganguli at IIT Delhi. After a short stint at teaching Physical Chemistry at Central University of Rajasthan, she moved back to the Nanoscale Research Facility, IIT Delhi as a scientist where she worked extensively on porous materials and their applications.

In 2014, she joined the Royal Society of Chemistry where she is currently the Editorial Development Manager and is responsible towards the development and implementation of the publishing strategy and related activities in India. She manages the journals & books and their growth in India. As a part of her role, she works quite extensively with the scientific community, various chemical societies, and researchers across various disciplines of Chemical Sciences.

Bio-Sketch of Chairperson
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Associate Dean of Research & Development (2020 - 2021): IISER Mohali

Academic Positions

Associate Professor (March 2016 - Till date): Department of Chemical Sciences, IISER Mohali
Assistant Professor (Jan 2010 - March 2016): Department of Chemical Sciences, IISER Mohali
Education
Post-doctoral Fellow (Jan 2006 - Sep 2006) - Texas A&M University, College Station, USA (With Prof. Brian T Connell)
Research Fellow (Jan 2004 - Dec 2005) - WestCHEM, University of Strathclyde, Glasgow, UK (With Prof. John A Murphy)
Research Associate (April 2003 - Oct 2003) - Indian Institute of Technology Kanpur, India (With Prof. Vinod K Singh)
Graduate Student (Ph.D, Aug 1997 - Mar 2003) - Indian Institute of Technology Kanpur, India (With Prof. Vinod K Singh)
M Sc Applied Chemistry (Aug 1995 - Apr 1997) - Anna University, Chennai
Industrial Experience
Scientist (Nov 2006 - Dec 2009), Integrated Product Development, Dr Reddy's Laboratories Ltd, Hyderabad, India.

Awards & Recognitions

Selected for the Bronze Medal from the Chemical Research Society of India (CRSI) for the year 2022.
Appointed to the Editorial Board of "Resonance" journal (2020 -).
Appointed as a CRSI Local Chapter Convener for Chandigarh/Amritsar Region by the Chemical Research Society of India (CRSI).

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
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Dr. Saptarshi Mukherjee is presently a Professor at the Department of Chemistry, Indian Institute of Science Education and Research (IISER) Bhopal. He did both his BSc and MSc from the Jadavpur University and carried out his doctoral research at the Indian Association for the Cultivation of Science, Kolkata under Professor Kankan Bhattacharyya on Time-Resolved Laser Spectroscopy. He then moved to the Bowling Green State University, Ohio for his post-doctoral research with Professor H. Peter Lu on Single Molecule Spectroscopy. He returned to India in late 2008 and joined the Department of Chemistry IISER Bhopal as an Assistant Professor where he still continuing.

Professor Mukherjee's research interests include ultrafast and single molecule spectroscopy of luminescent metal nanoclusters and self-assembled systems having biological relevance. He is the recipient of the INSA Young Scientist Award, CRSI Young Scientist Award, CRSI Bronze Medal and has been a Core and Founding Member of Indian National Young Academy of Sciences (INYAS). Professor Mukherjee is a Fellow of the National Academy of Sciences, Allahabad and is a Senior Editor of Chemical Physics Impact, a journal published by Elsevier. He has also served IISER Bhopal as its first Deputy Director.

Publications:

1. DNA Templated Modulation in the Photophysical Properties of a Fluorescent Molecular Rotor Auramine O by Varying DNA Composition. *J. Phys. Chem. B*, **2022**, *126*, 2658.
2. White Light Generation Through L-Ascorbic Acid Templated Thermo-Responsive Copper Nanoclusters. *ACS Sustainable Chemistry & Engineering*, **2022**, *10*, 1379.
3. Effect of Protecting Groups on Luminescent Metal Nanoclusters: Spectroscopic Signatures and Applications. *Chem. Commun.*, **2022**, *58*, 29.
4. Role of Small Moiety of a Large Ligand: Tyrosine Templated Copper Nanoclusters. *J. Phys. Chem. Lett.* **2021**, *12*, 3266.
5. Differentiating Least Stable Single Nucleotide Mismatch in DNA via Metal Ions Mediated Base Pairing and Using Thioflavin T as an Extrinsic Fluorophore. *J. Phys. Chem. Lett.* **2021**, *12*, 2547.

Bio-Sketch of Chairperson
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M.Sc. in Chemistry from the Indian Institute of Technology Delhi, New Delhi, India (2001).
B.Sc. (Honours) in Chemistry from the University of Calcutta (Ramakrishna Mission Vidyamandira, Belur Math), Kolkata, India (1999).

PROFESSIONAL EXPERIENCE

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Technical University, Kaiserslautern May – June 2012
Visiting Scientist
Indian Institute of Science Education and Research, Kolkata, India January 2011-present
Professor, Department of Chemical Sciences
Indian Institute of Science, Bangalore, India June 2009-December 2010
Indian Institute of Science Centenary Postdoctoral Fellow (Inorganic and Physical Chemistry Department)
Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany April 2006-June 2008
Postdoctoral research scientist (computational and theoretical biophysics)

AWARDS & RECOGNITION

Awarded Max-Planck Institute doctoral and postdoctoral fellowship, IISc Centenary PDF, Editorial Board Member of Scientific Reports, IISER Kolkata Senate Member

SELECTED PUBLICATIONS

(Citations: 2590, *h-index* = 27)

1. S. Bose, S. Dutta, **D. Koley***, "*Entering Chemical Space with Theoretical Underpinning of the Mechanistic Pathways in the Chan-Lam Amination*", *ACS. Catal*. **2022**, *12*, 1461-1474.
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5. M. M. Guru,† S. De,† S. Dutta, **D. Koley***, B. Maji*, "*$B(C_6F_5)_3$-Catalyzed Dehydrogenative Cyclization of N-Tosylhydrazones and Anilines via a Lewis Adduct: A Combined Experimental and Computational Investigation*", *Chem. Sci.* **2019**, *10*, 7964-7974 (**Selected for Synform**)
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Substrate induced catalyst formation under non-equilibrium conditions

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Abstract:
There remain critical gaps in our understanding of the emergence of functional biopolymers in the origins of Earth's biosphere. For instance, extant proteins, evolved over millions of years, carry out an impressive array of responsibilities, from catalysis and molecular recognition to motility and compartmentalization. One of the major goals of our lab is to investigate the possible origins of advanced enzymatic functions from folds of short peptide based paracrystalline phases. Further, we are excited about understanding the non-equilibrium structures of living systems.[1-6] I will show our recent discoveries of simple chemical systems that can be substrate-driven to access higher energy self-assembled states, just as seen in natural microtubules. Further, I will attempt to sketch our aims of developing self-assembled autonomous materials that can show temporal control of functions.[5,7-10]

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8. S. Ahmed, A. Chatterjee, K. Das and D.Das* Chemical Science 2019 10 7574-7578
9. S. Bal, K. Das, S. Ahmed and D.Das* Angew. Chem. Int. Ed. 2019 58 244
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Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

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Dibyendu Das is an Associate Professor in the Department of Chemical Sciences of Indian Institute of Science Education and Research (IISER) Kolkata, West Bengal, India. He received his MSc degree in Organic Chemistry at the University of Calcutta (India) (2005), PhD in Supramolecular Chemistry at IACS Kolkata (Thesis 2010) and postdoctoral training at the Emory University, USA. From Jan 2017, Dibyendu is leading an interdisciplinary group that focuses on designing active and adaptive materials by harnessing non-equilibrium self-assembly and exploring the functional materials under the purview of systems chemistry. His lab is invested in mimicking how living systems work from the perspective of the emerging and young field of systems chemistry.

Awards and Distinctions

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

A chemogenomic probe for determining mobile Zn(II) concentration and pro-drug activation in pancreatic β-cells

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Abstract: Zinc, the second most abundant essential transitional metal, has catalytic, structural, and regulatory functions in an estimated 3,000 human proteins affecting almost any aspect of cellular biology.1 The concentration of Zn(II), both bound and labile, vary across various cell type in the human body. The concentration of Zn(II) is tightly regulated. In blood, the concentration of Zn(II) is 12-16 μM and they are chelated or protein-bound. However, in β-cell, the concentration of mobile Zn(II) is abnormally high, up to several mM. These pancreatic β-cells are responsible for the biosynthesis, storage, and secretion of the right amount of insulin in our body. The total Zn2+ content of the mammalian pancreas is significantly higher than in other cell types. Among all the cell types in the pancreas, the β-cells have an unusually high Zn(II) concentration up to ~30 mM, among which ~100 μM of which is loosely bound. However, the cytosolic Zn(II) concentration in most cells is ~400 pM and the concentration in plasma and interstitial fluid is ~1 nM. Similar to other cell types, free cytosolic Zn(II) concentration in beta-cells appears to be tightly regulated to maintain cytosolic Zn(II) concentration in a rather low range at about 400 pM. Although several methods are available for β-cell imaging and measurement of mobile Zn(II) concentration in β cells, they lack selectivity and specificity for β-cell. In this regard, we seek to design a chemogenatic probe for selective and accurate measurement of Zn(II) in β cells. To achieve the cell specific localization of the fluorophores, the HaloTag linker is attached to both the fluorophores. Once the HaloTag protein is expressed in the β-cell, the probe will form a covalent adduct with the HaloTag protein.

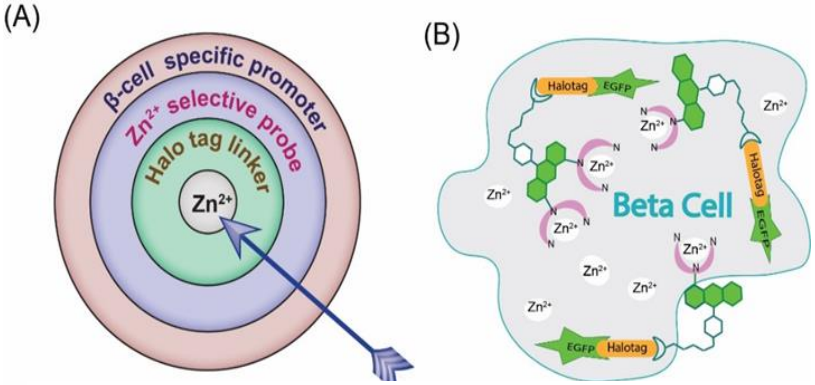

Figure 1*A*) A schematic representation showing the different layers of selectivity to the β-cell selective chemogenatic probe. **B**) A pictorial representation of the beta cell specific expression of HaloTag followed by covalent linkage formation with the Zn(II) selective fluorophore having the HaloTag linker

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Career Profile

May 2019 - till date: Assistant Professor, Dept of Chemistry, IISER-Bhopal

Nov 2016 - Mar 2019: *Research Fellow, Harvard Medical School and Broad Institute of MIT and Harvard, USA with Prof. Amit Choudhary

Apr 2014 - Dec 2015: Post-Doctoral Researcher, Dept of Organic Chemistry, Weizmann Institute of Science, with Prof. Rafal Klajn

July 2013: Integrated PhD, Dept of Inorganic and Physical Chemistry, IISc, Bangalore, Supervisor: Prof. G. Mugesh

July 2006: B.Sc., Jadavpur University, Kolkata

Raji Reddy Chada

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Dr. Raji Reddy has obtained M. Sc. from Osmania University in 1997. After completion of Ph. D. at CSIR-Indian Institute Chemical Technology in 2002, he moved as a post-doctoral fellow to University of South Florida, Tampa, USA (2002) and subsequently to University of Mississippi, USA (2002-2005). He returned to India in 2005 and joined as a principal scientist in Sai Life Sciences, Hyderabad. After one year, he joined CSIR-IICT, Hyderabad as a scientist at the Department of Organic Synthesis & Process Chemistry and presently working as a senior principal scientist.

His research interests are both fundamental and applied research, include (i) the chemistry of propargylic alcohols towards the synthesis of heterocycles and carbocycles; (jj) enyne-assisted reactions towards the synthesis of polyaromatic hydrocarbons (PAHs) and bio-active natural alkaloids; (iii) Process development of APIs.

Representative accomplishments are: processes for Favipiravir, Remdesivir, (*S*)-Pregabalin, key fragment of Erubulin mesylate and TLR 7/8 agonist molecule, used as an adjuvant in COVAXIN® (COVID-19 vaccine) have been developed and transferred to pharmaceutical organizations.

He is a recipient of CSIR-Technology Award-2021, NASI-Reliance Industries Platinum Jubilee Award-2020, CSIR-Technology Award-2020, CRSI Bronze Medal-2018, CDRI–Drug Research Excellence Award-2017, Dr. A K Singh Memorial-Young scientist award-2014, AVRA-Young scientist award-2011 and A P Akademi-Young scientist award-2007.
He is also Fellow of Telangana Academy of Sciences – 2019.

He is an author of 148-publications, 10-patents, 3-review articles and 2-book chapters. Under his supervision 24-Students have been awarded Ph. D. degree. Presently, 12-research fellows are working for their Ph. D. He has also supervised 20-Master students for their dissertation.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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Nanozyme: An Interdisciplinary Approach

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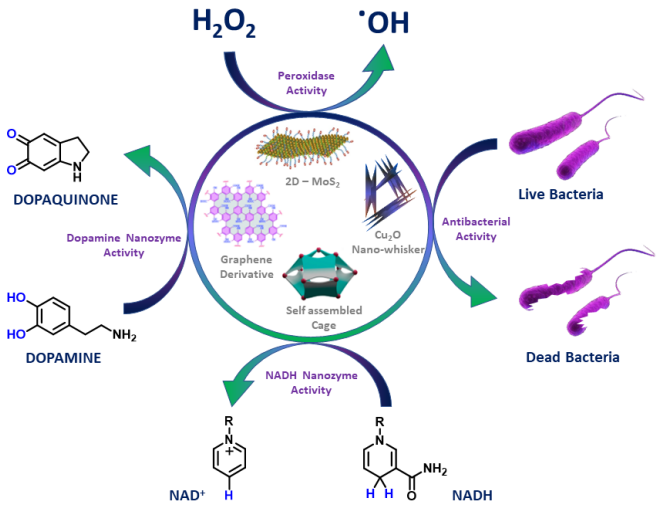
Abstract:
Nanozymes are materials/macromolecules with inherent enzyme-like characteristics. Since the landmark paper on nanozymes was published in 2007 based on iron oxide nanoparticle,[1] various types of nanozymes have been growing over the past decade because of their advantages compare to natural enzymes such as low stability, high cost, and difficult storage. Nanozymes were mainly conceptualized in interdisciplinary fields of material science, chemistry, biology and medicine. In our group, we mainly capitalize the nanozyme activity towards the development of antimicrobial agents. We have explored the peroxidase-like activity of transition metal dichalcogenides which was extended towards highly effective antimicrobial activity in presence of H_2O_2. We have also explored the role of functionalization, defects and doping in those materials for better understanding regarding the 2D-MoS_2 based nanozyme activity.[2-4] We have also explored the nanozyme activity in other materials such as graphene like system and macromolecular cages.[5,6] In a collaborative study we have used self-assembled Pd-coordinated macromolecular cage as photoregulated oxidase-like nanozyme to kill pathogenic bacteria.
Over the past decade, several research groups around the world are working on nanozymes using various types of nanomaterials. Nanozymes have great potential from in vitro detection to in vivo monitoring and many other catalytic applications in the future. But for the detail understanding and sustainable applications, required extensive collaborative effort in theoretical mechanistic understanding, preparation of hybrid materials, biological applications towards in vitro to in vivo etc.



Nanozyme activity of various nanomaterials/macromolecules.

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4. Ali, S. R.; De, *ACS Appl. Mater. Interfaces*, Accepted.
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6. Pandit, S.; De, M., *Nanoscale Adv.* **2021**, *3*, 5102-5110.

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Mrinmoy De received his M.Sc. from Indian Institute of Technology, Bombay, his Ph.D. from University of Massachusetts at Amherst under the supervision of Prof. Vincent M. Rotello and was a CCNE and NSEC postdoctoral fellow at Northwestern University. Since 2014 he has been at the Indian Institute of Science, Bangalore, where he is an associate professor at department of organic chemistry. His research focuses on the preparation various nanomaterials and their application towards development of nanoantibiotics, nanozymes, sensors and photocatalysis.

Finetuning electrophiles reactivity to induce target selectivity

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Abstract:
Rational drug design in covalent therapeutics and the emergence of powerful chemoproteomics platforms for target identification proved to be highly successful in identifying several unique therapeutic candidates in the past couple of decades. Despite the sharp rise in the knowledge base of the field, the off-target effects associated with the non-selective reactivity of electrophilic molecules have been a roadblock to the development of selective covalent therapeutics. The unmet need in this field is to understand the reactivity profiles of electrophilic warheads with nucleophilic amino acids and introduce selective reactivity in them. Isatoic anhydride (IA) is a potential electrophile with a capacity to react with nucleophilic amino acids with the release of thermodynamically more stable carbon dioxide during its modification. Here we show that incorporating appropriate chemical handles in the IA scaffold tips the selectivity balance between thiol (cysteine) or amine (lysine) nucleophiles in vitro and with recombinant proteins. Further, we demonstrate the molecules' propensity to modify cellular proteome using activity-based protein profiling experiments with HEK cell lysate and its applicability as protease inhibitors. This is a promising start for modulating electrophiles to imprint target selectivity at the stage of covalent modification

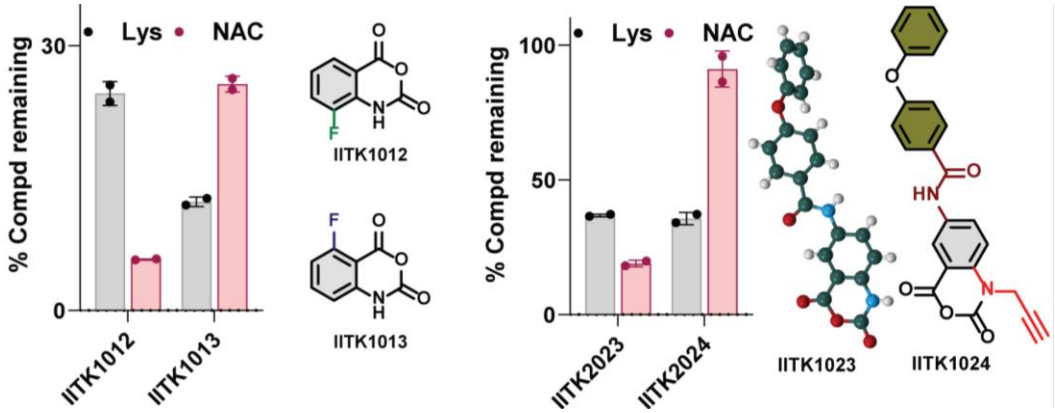

Figure 1. Finetuning the reactivity of IA-derivatives with appropriate chemical handles

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Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

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Career Profile, significant awards/achievements and representative publications

Area of Specialization: Chemical Biology

Awards:

1. Har-Gobind-Khorana Innovative-Young Biotechnologist Award (IYBA)-2019
2. Young Scientist Award-Chemical Research Society of India (CRSI)-2019
3. Associate member of Asian Chemical Biology Initiative (2019)
4. Director's Distinguished Postdoctoral Fellowship with a research grant, Los Alamos National Lab, USA (2018)

Publications:

1. J Sax, SN Hershman, Z Hubler, D Allimuthu,… DJ Adams, *ACS Chem Biol*, **2022**, Just Accepted
2. J Sax, SN Hershman, Z Hubler, D Allimuthu,… DJ Adams, *bioRxiv*, **2022**, doi: https://doi.org/10.1101/2022.06.21.497032
3. JL Sax, Z Hubler, D Allimuthu, DJ Adams, *ACS Chem Biol* **2021**, 16 (7), 1288-1297
4. Z Hubler, RM Friedrich, JL Sax, D Allimuthu, … , DJ Adams, *Cell Chem Biol*, **2021**, 28 (6), 866-875
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6. D Allimuthu, Z Hubler,… DJ Adams, *Cell Chem Biol* **2019**, 26 (4), 593-59
7. Z Hubler, # D Allimuthu, # ,…DJ Adams, *Nature*, **2018**, 560 (7718), 372-376 (# Co-first authors)

Bio-Sketch of Chairperson
FORCE-IICS Meeting during28th– 31stJuly, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

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omepage: http://www.iitrpr.ac.in/PBGroup/

Career Profile:

2016-till date Associate Professor, Department of Chemistry, IIT Ropar.
2010-2016 Assistant Professor, Department of Chemistry, IIT Ropar.
2007-2009 Postdoctoral Fellow, Purdue University, U. S. A.
2005-2007 Postdoctoral Fellow, RWTH-Aachen University, Germany.
2002-2004 Senior Research Fellow, CSIR, India.
1999-2002 Junior Research Fellow, CSIR, India.

Significant awards/achievements

2021 CRSI Bronze medal
2010-2013 DST young Scientist Award scheme
2007-2009 NIH post-doctoral fellow
2005-2007 DFG post-doctoral fellow
1999-2005 CSIR JRF and SRF

Representative publications

1. Pankaj Kumar, Navpreet Kaur, Rakesh Kumar and Prabal Banerjee,* "α,β-Unsaturated Carbonyls for One-Pot Transition-Metal-Free Access to 3,6-Dihydro-2H-Pyrans" *J. Org. Chem.***2022**, *87*, 7167-7178.
2.Debarshi Saha, Irshad MaajidTaily, Nakshatra Banerjee and Prabal Banerjee,* "Electricity Mediated [3+2]-cycloaddition of *N*-sulfonylcyclopropanes with Olefins via *N*-centered Radical Intermediates: Access to Cyclopentane Analogs" *Chem comm.*, **2022**, *28*, 5459-5462.
3. Irshad MaajidTaily, Debarshi Saha and Prabal Banerjee*, "Direct Synthesis of Paracetamol via Site-Selective Electrochemical Ritter-type C-H Amination of Phenol" *Org. lett.*, **2022**, *24*, 2310-2314.
4. Debarshi Saha, Irshad MaajidTaily, Sumitra Naik and Prabal Banerjee,* "Electrochemical Access to Benzimidazolone and Quinazolinone Derivatives via in situ Generation of Isocyanates" *Chem. Commun*., **2021**, *57*, 631-634.
5.Pankaj Kumar, Raghunath Dey and Prabal Banerjee,* "Exploitation of Cyclopropane Carbaldehydes to Prins Cyclization: Quick Access to (E)-Hexahydrooxonine and Octahydrocyclopenta[b]pyran", *Org. Lett.* **2018**, *20*, 5163-5166.

Abstract - Invited Lecture
FORCE-IICS Meeting during 28th – 31st July, 2022
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Potential use of beta-carboline derivatives as agents for treating pain

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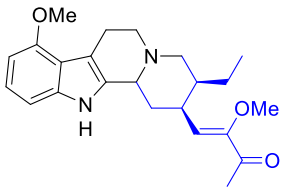
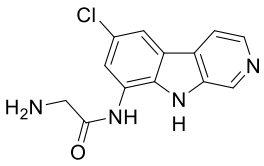
Abstract:
Pain, both acute and chronic, affects millions of people across the globe. Whereas Neuropathic pain is usually chronic, arising from progressive nerve disease, traumatic nerve injury, or infection, non-neuropathic pain (nociceptive pain) is typically due to somatic injury or illness. Treatment of intense and chronic pain requires the use of opioid analgesics but like every drug class, opioids also have adverse effects viz. sedation, dizziness, nausea, vomiting, constipation, physical dependence, tolerance, and respiratory depression. Consequently, there have been several efforts to discover novel compounds targeting known pain targets and explore emerging targets for pain treatment, which were reviewed recently.[1]

The β-carboline-based compounds are known to elicit a wide variety of bioactivities including alleviation of pain. Mitragynine (**1**), a β-carboline alkaloid is the major constituent of M. speciosa leaves, which has an opium-like effect and coca-like stimulating effect. Its analgesic and antitussive properties are comparable to codeine but unlike classic opioids, it does not produce respiratory depression.[2] Experimental evidence suggests that mitragynine binds preferably to μ-opioid receptors and κ-opioid receptors. The β-carboline derivative 6-chloro-8-(glycinyl)-amino-β-carboline (**2**) shows potent inhibitory activity of Nitric oxide implicated as a key factor in the pathogenesis of neuropathic pain.[3] Another report describes the β-carboline derivative (**3**) as a potent analgesic.[4] During our work exploring the medicinal chemistry of fused- β-carbolines, we have discovered a new β-carboline (**4**) with potent KOR agonist activity which may be used as a possible pain-relieving agent. Some of the results from our study will be presented and discussed.



Mitragynine, 1



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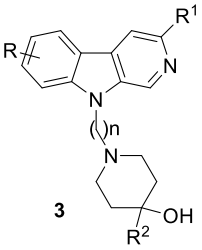

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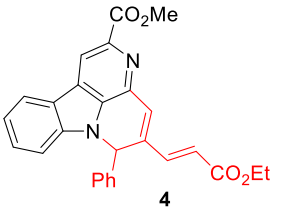

4
EC_{50} of **46±19 nM** @KOR

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5. Yadav, V. D.; Kumar, L.; Kumari, P.; Kumar, S.; Singh, M.; Siddiqi, M. I.; Yadav, P. N.; Batra, S. *ChemMedChem* **2021**, *16*, 1917.

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Sanjay Batra completed his Ph.D. in 1993 from the Medicinal and Process Chemistry Division at Central Drug Research Institute, Lucknow. He joined as faculty in the same department in 1995 and is presently working as Chief Scientist. In between November 2000 to November 2001, he worked as visiting scientist at the Chemistry Department, University of Mississippi, Oxford. He has made significant contributions in the area of medicinal and organic chemistry with special emphasis on the development of new drugs for neglected diseases. Two molecules one each for treating Visceral Leishmaniasis and Neuropathic pain (biased KOR agonist) from his research group are undergoing advanced IND enabling studies. He has also contributed to obtaining the IND permission for conducting clinical trials of a new antithrombotic compound that was licensed to the industry last year. He has more than 150 research publications, 17 review articles, and 3 book chapters to his credit.

Research Interests: His research interests include the development of chemistry associated with Morita-Baylis-Hillman adducts, transition metal and iodine-catalyzed reactions, and heterocyclic chemistry.

Awards and Honours: He is a fellow of the Indian National Science Academy and a Fellow of Royal Society of Chemistry. He is the recipient of Bronze medal from the Chemical Research Society of India (CRSI). He is a member of the International Advisory Board of *ChemMedChem* (Wileys publication). He has earlier served as Associate Editor for RSC Advances (2015-2017) and Chief Editor of Anti-Infective Agents (Bentham Publications (2011-2017).

Photoredox Catalyzed Single C–F Bond Activation

Indranil Chatterjee*
Department of Chemistry
IIT Ropar
(Email: indranil.chatterjee@iitrpr.ac.in)

Abstract:

Recent times have witnessed the robustness of visible-light-mediated transformations due to their cost-efficiency, convenience, and environmental friendliness. These are generally operative via radical pathways with metal or metal-free conditions, enriching the chemistry to synthesize various molecular architectures.

By using photoredox catalysis, the divergent reactivity of α,α-difluoromethyl ketone radical species with acrylamides and olefins will be discussed for the synthesize of difluoromethane containing value-added molecules.

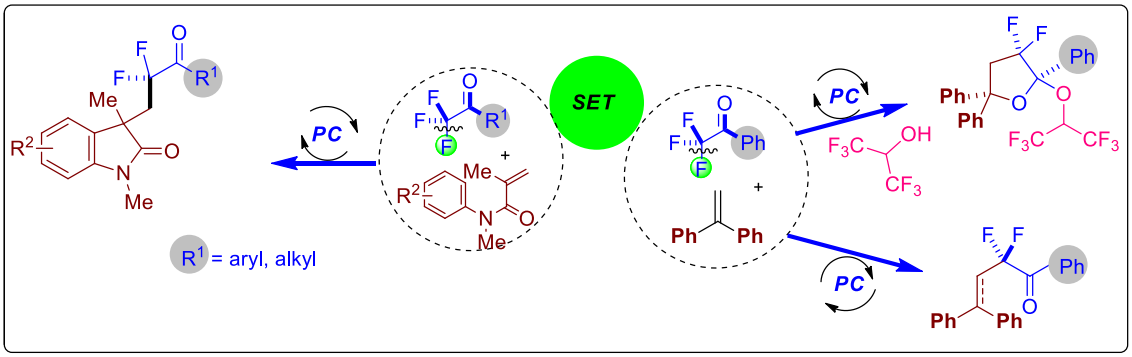

Figure 1: Activation of single C–F bond using visible-light photoredox chemistry.[1]

References and Notes:

[1] a) S. Ghosh, Z.-W. Qu, S. Pradhan, A. Ghosh, S. Grimme, and I. Chatterjee, *Angew. Chem. Int. Ed.* **2022**, *doi.org/10.1002/ange.202115272*; b) S. Ghosh, I. Chatterjee *unpublished work.*

Abstract - Invited Lecture

FORCE-IICS Meeting during28th– 31stJuly, 2022

…Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

Name Indranil Chatterjee

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Recent Picture

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Dr. Indranil Chatterjee obtained his B.Sc. from Calcutta University, India in 2006, and then he moved to IIT Kharagpur for his M.Sc. study. In 2008 he moved to Germany for his Ph.D. study at Westfälische Wilhelms-University Muenster under the guidance of Prof. Dr. Armido Studer, where his studies centred on catalytic asymmetric cycloaddition reactions. After finishing his Ph.D. study in November 2011, he joined as a Postdoctoral fellow with Prof. Paolo Melchiorre in ICIQ, Tarragona, Spain in March 2012. His area of research mainly focused on new organocatalytic cascade reactions. After that from 2014 to 2016 he did another Post-Doc with Prof. Martin Oestreich at the Technische Universität Berlin, concentrating his research on Lewis acid catalysis. Since December 2016 he is holding a position of Assistant Professor at the Indian Institute of Technology Ropar, India.

Details of any fellowship/awards/honors

(i) National Scholarship in Secondary and Higher Secondary exam. (2000 & 2002).
(ii) Ph.D. scholarship of the International Graduate School of Chemistry (GSC-MS), University of Muenster, Germany (2008-2011)
(iii) Postdoctoral Fellowship at ICIQ, Tarragona, Spain (2012-2014)
(iv) Cluster of Excellence UniCat Fellowship for Postdoctoral Research at Technical University Berlin, Germany (2014-2016)
(v) Institute Best Teaching Award (2020).
(vi) Thieme Chemistry Journal Award, 2022.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

Dr. Amit Kumar
Associate Professor
Department of Chemistry
Indian Institute of Technology Patna
Bihta, Patna, Bihar.

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E-Mail: amitkt@iitp.ac.in

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

Education:

- M. Sc. Delhi University: **2002**
- Ph. D. IIT Kanpur, India: **2008**

Postdoctoral Fellow*:*

- City University of New York, USA: **2008-2009**
- University of Konstanz, Germany: **2010-2012**

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

Publications: 45

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

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Biomimetic Total Synthesis of Marine Alkaloids

Rajesh Viswanathan*

Department of Chemistry and Biology

Indian Institute of Science Education and Research, Tirupati, AP, India,

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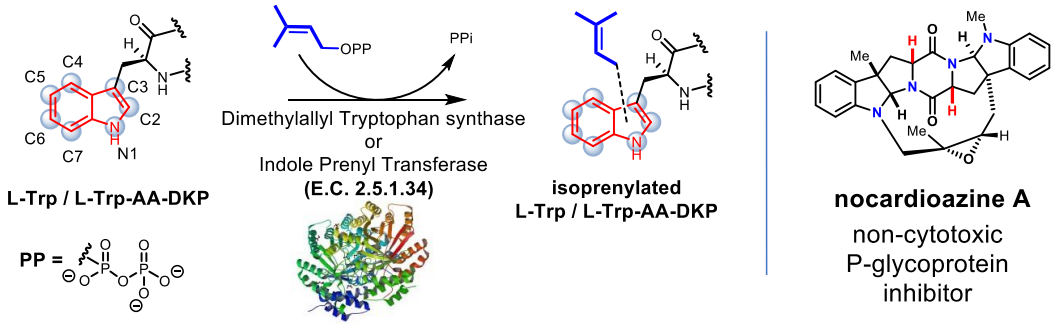
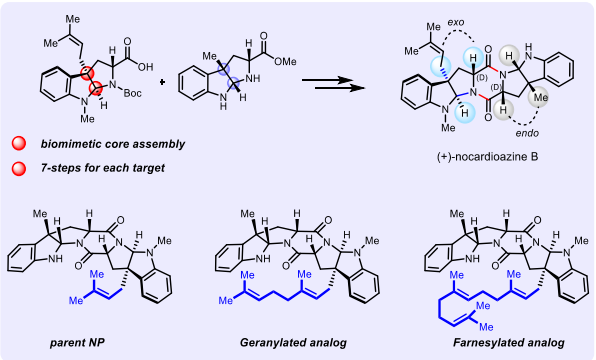
Abstract:

With rising cases of resistance to existing anticancer agents, there is a dire need to identify novel bioactives, as new-age therapeutics. The presentation will illustrate direct biomimetic functionalization of natural products (from marine and plant origin) that offers rich diversity of complex molecules. Their biomimetic total synthesis helps in building pharmacophores for biological evaluation. The talk will highlight recent advances on the total synthesis of (+)-nocardioazine alkaloids and their analogues (see Figure below). Nocardioazines are anti-cancer natural products that inhibit p-glycoprotein-mediated (Pgp) drug efflux. Synthetic pathway involves: Regio-and-Stereoselective Tryptophan prenylations, Cope rearrangements, pyrroloindoline construction; Pictet-spengler cyclizations and selective indole-C3/C2-functionalizations. These afford several non-toxic *P*-glycoprotein inhibitors, as leads. Ongoing biosynthetic studies on plant-derived *Trichopus* natural products afford new sources of antibiotics.

Biomimetic Studies of Natural Products



Highlights of Recent Studies



- Enables direct isoprenylation
- Modular assembly – 7 steps (shortest)
- Stereoselectivity for prenylation > 19:1 (^{1}H)
- Minimal protecting groups
- Overall yields ranging: 13.9 % to 23.6%
- Spectral characterization through ^{1}H; ^{13}C; COSY, ROESY, NOESY, HMBC, HSQC & HRMS
- Synthetic pathway provides easy access to P-gp inhibitors as leads

JOC **2014**, *79*, 10049; *ACS Synthetic Biology*, **2016,** *5*, 547; *OBC*, **2015,** ***13***, 7177;
ACS Omega. **2021,** *16*, 10840; *Nature Commun.* **2022**, *In revision*
J. Org. Chem. **2022**, *In press.*

Bio-Sketch of Speaker

Rajesh Viswanathan
Associate Prof. and Associate Dean

IISER Tirupati, India

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Homepage: https://rvresearch.weebly.com/

Career Profile:

M.Sc. IITK (Prof. Iqbal); Ph. D.: Indiana Univ. Prof. Johnston and Post-Doc: Univ. of Utah (Prof. Poulter)

- Associate Dean, Academics, IISER Tirupati
- Frank Hovorka Assistant Professor of Chemistry, CWRU, Cleveland, OH.
- Scientific Oversight Board Member, Small Molecule Drug Discovery Core; Case Western Reserve University, Cleveland, OH.
- Consultant for Chemical Operations, Gingko Bioworks: Synthetic Biology-based fine chemical production company, Boston, MA, USA.
- Faculty Excellence Award – Office of Inclusion, Diversity and Equal Opportunity, Case Western Reserve University.
- Outstanding Faculty Member: Gamma Sigma Alpha.
- Co-Investigator, Synthesis and Analytical Chemistry core, Program Project Grant, National Institutes of Aging (NIH P01 Grant)
- SERB-funded Chemical Biology Investigator, IISER Titupati.
- National Science Foundation grant awardee. Title: "Biosynthesis of Diketopiperazine Natural Products from Aminoacyl-tRNAs".

Significant Publications:

Biomimetic Total Synthesis of (+)-Nocardioazine B and analogs, *JOC, in Press.*

Bioinspired brØnsted acid-promoted regioselective tryptophan isoprenylations. *ACS Omega,* **2021,** *6,* 10840-10858.

Biocatalysts from cyanobacterial hapalindole pathway afford antivirulent isonitriles against MRSA. *Journal of Biosciences*, **2021**, *46* (2).

Two distinct cyclodipeptide synthases from a marine actinomycete catalyze biosynthesis of the same diketopiperazine natural product *ACS Synthetic Biology*, **2016,** *5*, 547–553

Structure-guided synthesis and mechanistic studies reveal sweetspots on naphthyl salicyl hydrazone scaffold as non-nucleosidic competitive, reversible inhibitors of human ribonucleotide reductase *J. Med. Chem.* **2018**, *61*, 666-680

Potent competitive inhibition of human ribonucleotide reductase by a non-nucleoside small molecule. *Proc. Natl. Acad. Sci. U. S. A.*, **2017,** *114*, 8241-8246.

Regioselective Cope rearrangement and prenyltransfers on indole scaffold mimicking fungal and bacterial dimethyl allyl tryptophan synthases *J. Org. Chem.* **2014**, *79*, 10049-10067.

Exploring the multiple conformational states of RNA Genome through network analysis

Debashree Chakraborty*
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Abstract:
The structural variation of RNA is often very transient and can be easily missed in experiments. Molecular dynamics simulation studies along with network analysis can be an effective tool to identify prominent conformations of such dynamic biomolecular systems. Here we describe a method to effectively sample different RNA conformations at six different temperatures (288 K, 303 K, 318 K, 333 K, 348 K and 363 K) by using relative orientations of the stems of the RNA molecule as the basis for the construction of a conformational network. This is a new methodology. This method gives us information about the prominent states of the RNA as well as the probability of the existence of different conformations and their interconnections during the process of evolution. The commonly used structural parameters such as RMSD, RGyr values often fail to give this information as many of the important details of the RNA might be neglected when we deal with the statistically averaged out data. We have taken SARS-CoV-2 RNA Genome as the system for this study.

It is seen that the prominent structures are in fact related at different temperatures and some of them have been observed to present at multiple temperatures. The timescale reported in the conformational dynamics matches well with the timescale reported for the hydrogen bond dynamics of G:C and A:U base pairs which shows the significance of this method. It is found that the ΔΔG calculated between 288 K and 363 K are found to be 10.31 kcal/mol (88 nt) which agrees well with the experimentally reported denaturation energy for similar RNA pseudoknot structure of E.coli α mRNA (~16 kcal/mol, 112 nt) determined by calorimetry/UV hyperchromicity and human telomerase RNA telomerase (4.5-6.6 kcal/mol, 54 nt) determined by FRET analysis.

References and Notes:

Singh O., Venugopal P. P., Mathur A., Chakraborty D.* *J. Mol. Graph. Mod.* **116**, 108264 (2022).

Bio-Sketch of Speaker

Name: Debashree Chakraborty

Designation: Assistant professor

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Homepage: http://chemistry.nitk.ac.in/faculty/debashree-chakraborty

Career Profile:
Dr. Debashree Chakraborty is a theoretical chemist and her research focuses mainly on the development and effective use of different computational techniques to solve the dynamics of biological systems. This is important for understanding the behaviour of the big biomolecular systems that have major applications in the medical field, such as neurogenetic disorder, necrotic cells, diabetes etc. She obtained her PhD from the Indian Institute of Technology Kanpur in 2011 and carried out postdoctoral research at the University of British Columbia, Vancouver, Canada and Insitut de Biologie Physico-Chimique, Paris, France. She began her independent research career as Assistant Professor at the Department of Chemistry, National Institute of Technology Karnataka, India, in 2015.

Significant Awards/Achievements: She is a recipient of Young Associate-Indian Academy of Sciences (2020-2023), SERB Women Excellence Award 2022, CRSI Bronze medal 2023.

Representative publications:

1) Epitope-Based Potential Vaccine Candidate for Humoral and Cell-Mediated Immunity to Combat Severe Acute Respiratory Syndrome Coronavirus 2 Pandemic.
B. K. Das and D. Chakraborty*, J. Phys. Chem. Lett., 11, 9920 (2020).

2) Preferential binding affinity of ions and their effect on structure and dynamics of water near antimicrobial peptide
Omkar Singh and **D. Chakraborty***, *J. Mol. Liq.*, **344**, 117789 (2021).

3) Structural and dynamical properties of water in surfactant-like peptide-based nanotubes: Effect of pore size, tube length and charge.
Dilip H. N. and **D. Chakraborty***, J. Mol. Liq., 323, 115033 (2021).

4) Dilip H. N. and **D. Chakraborty***, "Hydrophilicity of the hydrophobic group: Effect of cosolvents and ions", J. Mol. Liq., 280, 389-398, 2019.

5) **D. Chakraborty** and G. N. Patey, "How Crystals Nucleate and Grow in Aqueous NaCl Solution", J. Phys. Chem. Lett., 4, 573, 2013.

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

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Bio-Sketch of Speaker

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Kartik Chandra Mondal received his Ph. D in 2011 from Karlsruhe Institute of Technology (KIT) under the supervision of Professor Annie K. Powell. He worked on mixed 3d – 4f ion based single molecule magnets. After a short stay as a postdoctoral researcher in the same group he moved to University of Göttingen in October, 2011 – 2015. He has been appointed as an assistant professor at Department of Chemistry, IIT Madras at the end of 2015. Since then he has been working in the research areas given below. Dr. Mondal has coauthored more than 50 peer – reviewed publications in leading scientific journals.

Educational Qualification:

- 2011 – Ph. D from KIT, Karlsruhe, Germany
- 2007 - M. S from I. I. Sc. Bangalore, India.
- 2004 - B. Sc from RKM - Narendrapur, University of Calcutta, Kolkata

Research Interests:

- Carbene stabilized main group element or transition metal atom
- Radical, diradical and radicaloid
- Organometallic single molecule/ion magnet
- Organic catalysis by above mentioned species
- Theoretical calculations on stability, bonding aspects of unusual exotic species

Reversible Fluorescent Chemical Tools for Imaging Signal-Mediating Lipids

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Abstract:

Tracking the spatiotemporal dynamics of small molecules and ions which regulate key decision-making processes in living systems can provide critical insights into biological pathways in both normal and disease states. In this context, fluorescent chemical sensors that illuminate molecules of life have emerged as powerful tools. However, major challenges related to distinguishing similar molecules and inability to achieve reversible sensing have restricted live imaging to a chosen few bio-analytes. We have leveraged chemical recognition and secondary non-covalent interactions to develop reversible sensors that can capture a wide range of non-genetically encoded small molecules and ions in action. In this talk, I will highlight our work on the design and development of reversible fluorescent chemical sensors for imaging signal-mediating phospholipids.[1-3]

References and Notes:

1. Chandra, A.; Datta, A. *ACS Omega* **2022,** *7* (12), 10347-10354.
2. Kundu, R.; Chandra, A.; Datta, A. *Israel Journal of Chemistry* **2021,** *61* (3-4), 199-216.
3. Mondal, S.; Rakshit, A.; Pal, S.; Datta, A. *ACS Chemical Biology* **2016,** *11* (7), 1834-1843.

Bio-Sketch of Speaker

Ankona Datta
Associate Professor

Department of Chemical Sciences
Tata Institute of Fundamental Research

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Ankona received her B.Sc. and M.Sc. degrees in chemistry from the Indian Institute of Technology, Kharagpur in 2000. She did her graduate work on chiral water-soluble porphyrins for catalysis and recognition with Prof. John T. Groves at Princeton University (Ph.D., 2006). After graduating from Princeton, she joined as a postdoctoral scholar in the laboratory of Prof. Ken Raymond at the University of California, Berkeley, where she worked on macromolecular MRI contrast agents.

Since 2010 she is a faculty in the Department of Chemical Science at the Tata Institute of Fundamental Research, India. Her current research interests are in the fields of Chemical Biology and Molecular Imaging.

Honors/Awards

Eminent and Empowered Women Award for a Scientist, Women Graduates Union	2018
ACS Emerging Investigator in Bio-Inorganic Chemistry	2015

Representative Publications

1. Das, S.; Kapadia, A.; Pal, S.; **Datta, A**.*, Spatio-Temporal Autophagy Tracking with a Cell-Permeable, Water-Soluble, Peptide-Based, Autophagic Vesicle-Targeted Sensor. ***ACS Sensors*****, 2021,** *6* (6), 2252-2260.

2. Das, S.; Carmona, A.; Khatua, K.; Porcaro, F.; Somogyi, A.; Ortega, R.; **Datta, A.***, Manganese Mapping Using a Fluorescent Mn^{2+} Sensor and Nanosynchrotron X-ray Fluorescence Reveals the Role of the Golgi Apparatus as a Manganese Storage Site. ***Inorganic Chemistry,*** **2019,** *58* (20), 13724-13732.

3. Rakshit, A.; Khatua, K.; Shanbhag, V.; Comba, P.; **Datta, A.*,** Cu^{2+} selective chelators relieve copper-induced oxidative stress in vivo. ***Chemical Science,*** **2018,** *9* (41), 7916-7930.

Visible Light-mediated Reactions of Diazo Compounds

Namrata Rastogi*
Medicinal & Process Chemistry Division
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Abstract: The diazo compounds are one of the most potent classes of organic compounds in terms of their versatile reactivity profile considering their participation in 1,3-dipolar cycloadditions, ylide formation, Wolff rearrangement, C-H or X-H insertions etc.[1] The recent progress in the visible-light-mediated photochemical reactions of diazo compounds has further consolidated their position as one of the most valuable synthetic building blocks. The diazo compounds serve as precursors to free carbenes, ketenes, diazoalkyl radicals as well as carboxyl radical under visible light-mediated conditions.[2]

In this presentation, our research group's work on the photochemical reactions of diazo compounds catalyzed by organo-photocatalysts or organometallic photocatalysts will be discussed.[3-5] These reactions include organo-photocatalytic generation of enolate vinyl radicals and generation of diazoalkyl radicals in the presence of organometallic photocatalyst. The enolate vinyl radicals and diazoalkyl radicals were trapped by suitable substrates leading to the synthesis of various carbo/heterocyles such as naphthols, phenanthren-10-ols, phenanthridines, diazirines and tetrazoles (Figure 1).

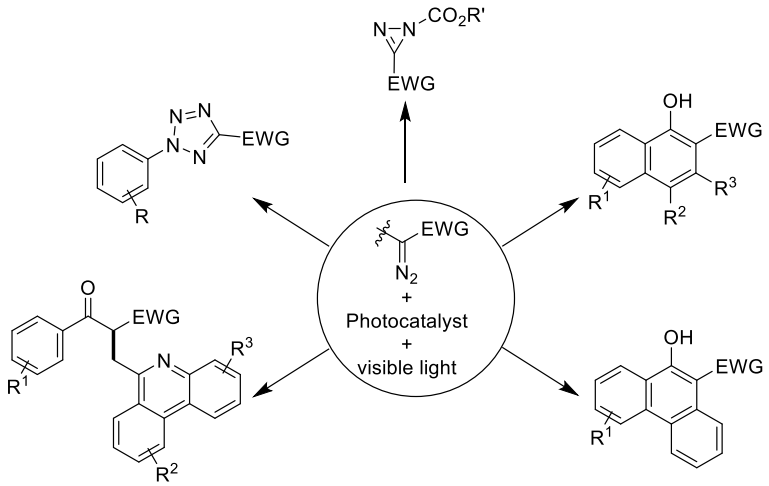

Figure 1

References and Notes:

1) Ford, A.; Miel, H.; Ring, A.; Slattery, C. N.; Maguire, A. R.; McKervey, M. A. *Chem. Rev.* **2015**, *115*, 9981-10080.
2) Durka, J.; Turkowska, J.; Gryko, D. *ACS Sustainable Chem. Eng.* **2021**, *9*, 8895-8918.
3) Nagode, S. B.; Kant, R.; Rastogi, N. *Org. Lett.* **2019**, *21*, 6249-6254.
4) Devi, L.; Pokhriyal, A.; Shekhar, S.; Kant, R.; Mukherjee, S.; Rastogi, N. *Asian J. Org. Chem.* **2021**, *10*, 3328-3333.
5) Pathak, J.; Srivastava, O.; Rastogi, N. *manuscript under preparation*

Bio-Sketch of Speaker

Dr. Namrata Rastogi

Principal Scientist

Medicinal & Process Chemistry Division

CSIR-Central Drug Research Institute

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Homepage: https://www.cdri.res.in/1788.aspx?id=1788

Career Profile:

Principal Scientist	March, 2020-till date (CSIR-CDRI, Lucknow)
Senior Scientist	March, 2016-March, 2020 (CSIR-CDRI, Lucknow)
Scientist	March, 2011-March, 2016 (CSIR-CDRI, Lucknow)
Senior Research Scientist	July, 2009-March, 2011 (Jubilant Biosys Ltd, Bengaluru)
Postdoctoral Research Associate	April, 2007-April, 2009 (University of Minnesota, USA)
Postdoctoral Research Associate	September, 2006-March, 2007 (IIT, Kanpur)
PhD	January, 2001-July, 2006 (IIT, Bombay)

Significant Awards/Recognitions:

- INSA-DFG Visiting Scientist, University of Regensburg, Germany-2014
- ISCB-Distinguished Women Scientist Award-2019 in the area of Chemical Sciences
- Member of International Advisory Board-Asian Journal of Organic Chemistry, 2020-2024
- Chemical Research Society of India (CRSI) Bronze medal-2022

Representative Publications:

1) Devi, L.; Kumar, P.; Kant, R.; Rastogi, N. *Chem. Commun.* **2022** *just accepted*
2) Pokhriyal, A.; Karki, B. S.; Kant, R.; Rastogi, N. *J. Org. Chem.* **2021**, *86*, 4661-4670.
3) Nagode, S. B.; Kant, R.; Rastogi, N. *Chem. Asian J.* **2020**, *15*, 3513-3518.
4) Nagode, S. B.; Kant, R.; Rastogi, N. *Org. Lett.* **2019**, *21*, 6249-6254.
5) Pokhriyal, A.; Karki, B. S.; Kant, R.; Rastogi, N. *Org. Biomol. Chem.* **2018**, *16*, 7152-7156
6) Pramanik, M. M. D.; Nagode, S. B.; Kant, R.; Rastogi, N. *Org. Biomol. Chem.* **2017**, *15*, 7369-7373.
7) Pramanik, M. M. D.; Rastogi, N. *Chem. Commun.* **2016**, *52*, 8557-8560
8) Chaturvedi, A. K.; Kant, R.; Rastogi, N. *J. Org. Chem.* **2016**, *81*, 11291-11296.
9) Chaturvedi, A. K.; Rastogi, N. *J. Org. Chem.* **2016**, *81*, 3303-3312.
10) Pramanik, M. M. D.; Chaturvedi, A. K.; Rastogi, N. *Chem. Commun.* **2014**, *50*, 12896-12898.

Bio-Sketch of Chairperson
FORCE-IICS Meeting during 28th – 31st July, 2022
…Anticipating Tomorrow's Science through Collaborative Ventures

Dr. Shaikh M. Mobin, FRSC
Associatre Professor
Department of Chemistry
IIT Indore
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Indore
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Dr. Shaikh accomplished his Bachelor's and Master's from Wilson College, University of Mumbai with major in Chemistry and PhD from Mumbai University in Chemistry. In 2012, he joined IIT Indore and presently working as an Associate Professor in Discipline of Chemistry. He had developed his research group working in wide area of research including Optical and electrochemical sensing, Solid-state structural reactivity, MOFs based Supercapacitors for energy storage, catalysis, sensing and bio-medical applications. Metal oxide nano-materials derived by employing metal complexes / MOFs as single-source molecular precursors is used for catalyst in organic transformation and electrocatalyst for water splitting. Design and synthesis of greener c-dots and their wide range of bioimaging and biosensing applications and Lead-Free solar cells are major area of focus by the group. Moreover, the research group designs and synthesizes small molecules as cellular organelles target and cell imaging.

Achievements:

- Fellow of Royal Society of Chemistry (FRSC).
- Recipient of Material Research Society of India (MRSI) Medal 2021.
- Fellow of Indian Chemical Society (FICS).
- Fellow of Maharashtra Academy of Sciences (FMASc).
- Dr Shaikh has been named as ***Golden Author*** by *Dalton Transaction*, Royal Society of Chemistry on occasion of 50th Volumes of Dalton Trans.
- Dr. Shaikh has been recognised as the Outstanding Reviewers for Dalton Transactions in 2018 (*Dalton Trans.*, 2019, ***48***, 4758-4758).
- Dr. Shaikh has been listed amongst highly prolific authors by ***Current Science***, (*CURRENT SCIENCE, VOL. 109, NO. 5, 10 SEPTEMBER 2015*) rivalling researchers from prestigious institutions such as CSIR-IICT, CSIR-NCL and IIT Kharagpur.
- Recognised among top 10 researchers in Chemistry in India by ***Careers 360*** (Most Outstanding Researcher Award, 2018) with a *h*-index of 57, more than 500 publications and ~14300 citations to date.
- Research work on novel dye for tracking lysosomes in live cell imaging covered by ***Free Press Journal*** Indore edition (April 14, 2018).

Abstract - Invited Lecture

FORCE-IICS Meeting during 28th – 31st July, 2022

...Anticipating Tomorrow's Science through Collaborative Ventures

Bio-Sketch of Speaker

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2017- **Associate Professor**
School of Chemical Sciences, NISER.

2013-2017 - **Reader-F**
School of Chemical Sciences, NISER.

2011-2016 - **Ramanujan Fellow (SERB)**
School of Chemical Sciences, NISER.

2011-2013 - **Assistant Professor**
School of Chemical Sciences, NISER.

2009-2011- **Alexander von Humboldt Research Fellow,** RWTH Aachen University, Aachen Germany. Advisor: Prof. Walter Leitner

2006-2008- **Dean of Faculty Postdoctoral Fellow** Weizmann Institute of Science, Israel. Advisors: Prof. David Milstein & Prof. Hadassa Degani

2005-2006- **Postdoctoral Fellow**
Weizmann Institute of Science, Israel.
Advisors: Prof. David Milstein &
Prof. Hadassa Degan

Areas of Research:

Chemistry of transition metal pincer complexes
C-H activation of alkanes, arenes and alkenes
Activation of small molecules
Metal catalyzed multi-component reactions
Lanthanides in catalysis and sustainable chemistry

Awards

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

Spin-State Switching in Dynamic Molecular Crystals

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Abstract:
The development of molecular materials that can be switched between two different spin states through the application of external stimuli is of great interest owing to their potential use in molecular devices and information technology.[1,2] This switching behavior can be triggered by different phenomena such as a charge/proton transfer, a change in the solid-state structure, or molecular orientation. When the *cooperativity* between spin centres is strong enough, a region of bistability might open, in which either of the two states can be found depending on the material's immediate past. This *memory* effect has been widely exploited in transition metal complexes. Some exciting recent discoveries[3-4] of spin-state switching in the transition metal complexes in presence of external perturbation would be discussed in this presentation.

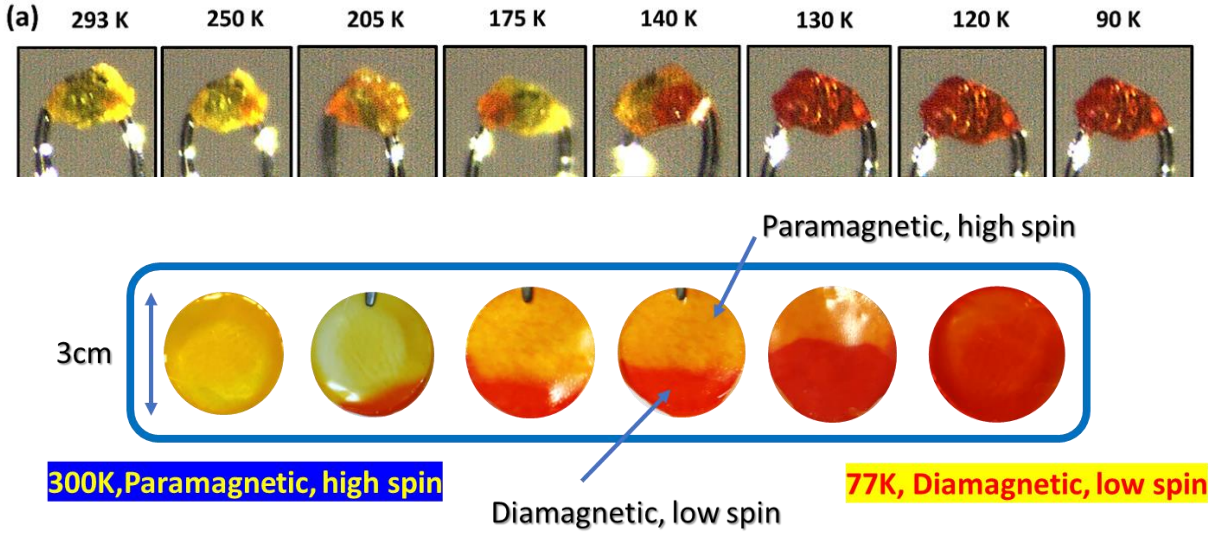

Figure: Dynamic behavior of spin-crossover crystals and their polymer nanocomposite

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Sanjit Konar received his Ph.D. from the Indian Association for the Cultivation of Science, Kolkata. After that, he worked as a postdoctoral fellow at the University of Notre Dame and Texas A&M University, College Station, TX, USA. He is a recipient of an Alexander von Humboldt Fellowship and has worked at Universität Bielefeld, Germany. Currently, he is working as a Professor at the Department of Chemistry, IISER Bhopal, India. His research revolves around molecular magnetism, switchable magnetic materials, and polyoxometalates. He has published 145+ peer-reviewed journal articles, having ~5400 citations and an H-index of 43. He currently serves as the international editorial board member of the Wiley journal European Journal of Inorganic Chemistry, MDPI journal Magnetochemistry and an associate editor of ACS journal Crystal Growth and Design.

How to harvest organic triplet energy at or above room-temperature?

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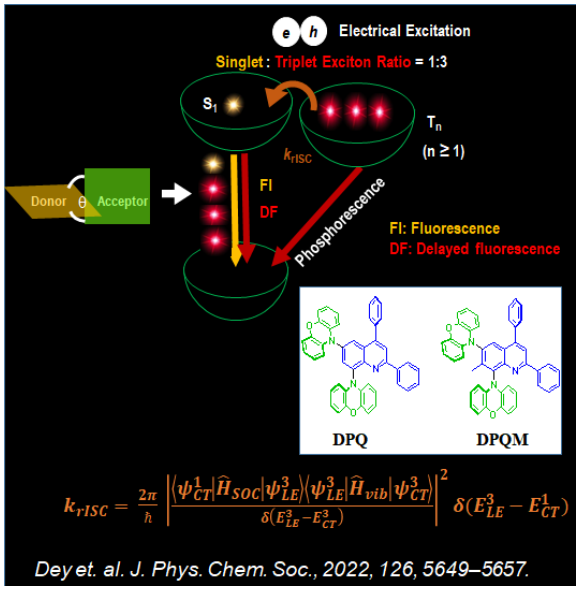
Abstract:
Borrowing an idea of delayed fluorescence, Perin (1929)[1], Lewis (1941)[2], Parkar (1961) and Hatchard (1968) in the two papers[3,4] proposed the idea of E-type delayed fluorescence in Eosin and Benzyl. This emission mechanism, now known as thermally activated delayed fluorescence (TADF) was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

Figure:



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Debdas Ray, associate professor of the Department of Chemistry, Shiv Nadar University, Delhi-NCR, has earned his Ph. D. degree (PI: Professor Parimal Kanti Bharadwaj) from Indian Institute of Technology Kanpur. His doctoral research work was based on the selective detection of biologically important metal ions using fluorescence signaling. He had also explored other research scopes outside India (France, USA, Japan), and significantly contributed to the groups. Presently, Dr. Ray is having more than ten years of experience in photophysics and photochemistry background. He has successfully applied various spectroscopic techniques to study and understand the excited state dynamics of molecular systems for triplet energy harvesting for OLEDs, data security, photosensitizer, and sensors. In India, he has developed a new research area of triplet energy harvesting via up-conversion of excited triplet state to singlet (i.e., thermally activated delayed fluorescence) state along with persistent-emission at ambient conditions.
His research outcomes have been published in highly reputed journals, and cited by high impact journals. Recently, he has invented "invisible ink" which had published in thirty four national and international newspapers. Recently, he has published two ACS articles (J. Phys. Chem. Lett.) in single volume, which is one of the rare achievements of his research activity (highlighted by ACS-live slide presentation). Furthermore, he has successfully developed a novel and un-explored route to allow efficient harvesting of triplet energy above RT.

Representative publications

(a) Dey, S.; Hasan, M.; Shukla, A.; Acharya, N.; Upadhyay, M.; Lo, S.-C.; Namdas, E. B.; Ray, D. *J. Phys. Chem*. C. **2022**, *126*, 5649–5657.
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(g) Bhattacharjee, I.; Acharya, N; Karmakar, S.; Ray, D. *J. Phys. Chem*. C, **2018**, *122*, 21589-21597.

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