Indo-German mini-Workshop 2022:
Complex Chemical Systems
(IGmW-CCS-2022)

OCTOBER 5, 2022

Department of Chemistry
IIT Madras

Message from the Head of the Department

Dear Colleagues and Participants:

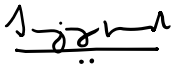
I invite you to Indo-German Workshop-2022 (IGW-CCS-2022), scheduled on October 5-8, 2022. This IGW-CCS-2022 is a unique event where German/European scientists and Indian scientists come together and spend time discussing and brainstorming their recent research findings. Department of Chemistry, IIT Madras, is happy and proud to organize this great event.

I urge faculty members, Ph.D. scholars, post-doctoral fellows, research associates, and M.Sc. students of the Department to participate in the event and utilize this rare opportunity to enhance their knowledge. One will undoubtedly benefit from the international event and also will be able to comprehend the overall research activities.

I want to record the sincere efforts of the organizing team in arranging this Indo-German Workshop-2022. After a break of two and half years, we look forward to getting together and having face-to-face interaction with the Indian and European scientists at this international event.

I wish you a successful and memorable Indo-German Workshop!

Best regards



Professor Sanjay Kumar
Head, Department of Chemistry
IIT Madras
INDIA

Message from the Organizers

We welcome you to Indo-German Workshop-2022: Complex Chemical Systems (IGW-CCS-2022), scheduled on October 5-8, 2022. This workshop will bring chemists from India and Germany/Europe under the thematic title of *Complex Chemical Systems*. IGW-CCS-2022 is expected to intensify scientific interaction among leading researchers in India and Germany/Europe. This IGW-CCS-2022 is an international event where more than ten German/European speakers and several Indian scientists come together to discuss their recent research findings.

It will enable researchers to identify areas where scientific collaboration might be possible to understand complex chemical systems better, developing new catalysts, value-added molecules mainly focused on healthcare & well-being, and new materials.

We are confident that this IGW-CCS-2022 will be a productive and memorable event.

With best regards

(Prof. G. Sekar)
Department of Chemistry
IIT Madras

Convener
IGW-CCS-2022

(Prof. Dr. Alexander Heckel)
Goethe Universität Frankfurt
Germany

German Coordinator
IGW-CCS-2022

October 5, 2022 (Wednesday)

Venue: IC&SR Auditorium, IIT Madras

Inaugural Function (2.30 – 3.00 PM)	**Welcome Address:** Prof. G. Sekar, IIT Madras **About IGW-2022:** Prof. Alexander Heckel, Goethe University-Frankfurt, Germany Prof. Sanjay Kumar, HoD Chemistry, IIT Madras Prof. Raghunathan Rengaswamy, Dean (GE), IIT Madras **Chief Guest address:** Prof. V. Kamakoti, Director, IIT Madras Ms. Michaela Küchler, German Consulate General Chennai **Vote of thanks:** Prof. G. Sekar
SESSION 1 (3.00 – 4.30 PM)	**Chairperson: Prof. S. Sankararaman (IIT Madras)**
3.00 – 3.30 PM	**Prof. Andreas Dreuw** (University of Heidelberg) *Quasi-Particles in Chemistry*
3.30 – 4.00 PM	**Prof. T. Pradeep** (IIT Madras) *Complexity in the Chemistry of Atomically Precise Clusters*
4.00 – 4.30 PM	**Prof. Alexander Heckel** (Goethe University-Frankfurt) *Regulation of Oligonucleotides in Time and Space*
4.30 – 5.00 PM	**TEA / COFFEE BREAK**
SESSION 2 (5.00 – 6.30 PM)	**Chairperson: Prof. K. Mangala Sunder (IIT Madras)**
5.00 – 5.30 PM	**Prof. Alakesh Bisai** (IISER Kolkata) *Nature Inspired Oxidative Strategies for Dixiamycins & Taiwaniadducts*
5.30 – 6.00 PM	**Prof. Nina Morgner** (Goethe University-Frankfurt) *Biomolecular complexes: required and unwanted assemblies – what can we learn with native mass spectrometry?*
6.00 – 6.30 PM	**Prof. Beeraiah Baire** (IIT Madras) *The Z-enaote assisted Meyer-Schuster rearrangement: An umpolung functionalization of propargylic alcohols*
7.30 PM	**DINNER @ Le Royal Méridien Chennai**

Chairpersons

Prof. Dr. S. Sankararaman
Professor

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Education:
1985 Ph.D. Department of Chemistry, University of Victoria, Victoria, Canada.
1981 M.Sc. Department of Chemistry, Indian Institute of Technology Madras, India.
Professional experience:
1985-1990 Postdoctoral Fellow, Dept. of Chemistry, University of Houston, TX, USA.
1991-1996 Assistant Professor, Department of Chemistry, IIT Madras, India.
1996-2000 Associate Professor, Department of Chemistry, IIT Madras, India.
2000-present Professor, Department of Chemistry, IIT Madras, Chennai, India.
Awards and Fellowships:
2020 Elected fellow of the Indian National Science Academy, New Delhi.
2017 Elected fellow of the Indian Academy of Sciences, Bangalore.
2010 Bronze medal, Chemical Research Society of India.
1998 Alexander von Humboldt (AvH) Fellowship.

Research interests are in the areas of synthetic acetylene and alkene chemistry, weak molecular interactions such as π–π and H-bonding, abnormal *N*-heterocyclic carbene complexes, photochemistry,organic redox flow batteries.

A new 2,3-dimethoxy-1,4-naphthoquinone redox anolyte for non-aqueous organic static redox battery.
P. Vallayil, K. Ramanujam, S. Sankararaman. Electrochemica Acta., **2022**, 407, 139889.

Conducting and superhydrophobic hybrid 2D material from coronene and pyrene.
J. S. Arya, M. K. Mahato, S. Sankararaman, E. Prasad, *J. Mat. Chem.C*, **2021**, *9*, 10324.

Which isomer is it, 1,2,5,6- or 1,4,5,8-tetrasubstituted cycloocta-1,3,5,7-tetraene? Synthesis of symmetrically tetrasubstituted cycloocta-1,3,5,7-tetraene derivatives.
S. Gadigennavar, M. Ranganathan, S. Sankararaman, *Org. Biomol. Chem*., **2020**, *18*, 9284.

Synthesis and application of 3,4,7,8-tetrakis-exo- methylenecycloocta-1,5-diene as a versatile Diels-Alder diene. Synthesis of V-shaped cyclooctatetraene fused acenes.
S. Gadigennavar, S. Sankararaman, *Org. Biomol. Chem*., **2020**, *18*, 6738-6744.

Prof. Dr. Mangala Sunder Krishnan
Professor Emeritus

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Dr. Mangala Sunder Krishnan is Professor Emeritus in the Department of Chemistry, IIT Madras from July 2022 after he completed more than 25 years of service as faculty member during which time, he was Professor for fifteen years. His primary areas of research are theoretical chemistry, molecular spectroscopy, nuclear magnetic resonance, computational chemistry, and quantum information processing. He was also a contributor as National Coordinator in the development of several programs of the Ministry of Education, Government of India since 2003 on digital content development and courses in engineering, arts and humanities, social sciences, science and technology through funded projects, namely National Programme on Technology Enhanced Learning (NPTEL), National Mission on Education through Information and Communication Technology (NMEICT), Study Web Actives for Young and Inspiring Minds (SWAYAM), India's Massive Open Online Courses (MOOCs) and Direct to Home SWAYAM Prabha (34 free educational channels 24/7). In addition, he has been an advisor to the E-learning Division, Ministry of Electronics and Information Technology, Government of India from 2006. He currently carries out a program of Digital Skills Academy in IIT Madras based on National Skills Qualification Framework and the national efforts on Future Skills Prime. The YouTube channel set up by him in 2007 (https://www.youtube.com/iit) for free access to all video lessons developed with the support of the Government has more than a billion views.

Seven graduate students have completed their Ph. D. programme with his help and guidance and currently he has two Ph. D. students. More than 30 M. Sc. Students have done their project with him for their master's degree. His research work consists of about 37 peer reviewed articles in leading international journals and more than 75 national and international conference presentations. As part of the digital initiatives he was involved, he has travelled extensively in India and abroad and has delivered more than 200 lectures so far. He is also active in the School Education sphere working with large number of teachers and parents through digital and learning initiatives such as Kuruvila Jacob Initiative and the Research Science Initiative, Chennai.

Dr. Krishnan is a native of Tirunelveli district, Tamil Nadu and obtained his degrees in Chemistry from Madurai (B.Sc.) and Madras Universities (M. Sc.). He was briefly employed in the Chemistry Division of Bhabha Atomic Research Centre, Government of India after successfully completing the training programme of the 23rd batch of Training School. Subsequently, he obtained his Ph. D. degree from McGill University, Montreal, Canada and was a post-doctoral fellow in the University of British Columbia in Vancouver, Université de Montréal in Montreal, and Queens University in Kingston, Canada before joining IIT Madras in 1996. He has had several visiting fellowships in India and McGill and was also a Visiting Professor in the Indian Institute of Science, Bangalore for brief periods. He received the "commendable Contributions to Digital Learning" award from the Hon. President of India (Late) Shri. Pranab Mukherjee in the year 2017. He was also the recipient of the Sterry Hunt Award in McGill for three years, 1984-1986 as one of the best laboratory teaching assistants.

Dr. Krishnan and his wife Mrs. Shailaja Iyer have two children, a son and a daughter. He enjoys reading published works in English and Tamil literature as well as history of the world and science, physics and chemistry in particular.

Invited Lectures

Prof. Dr. Andreas Dreuw
Professor

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Prof. Andreas Dreuw received his Ph.D. in Theoretical Chemistry from Heidelberg University in 2001. After a two-year postdoc at the UC Berkeley, he joined the Goethe University of Frankfurt first as an Emmy-Noether fellow and then as a Heisenberg-Professor for Theoretical Chemistry. Since 2011, Andreas Dreuw holds the chair for Theoretical and Computational Chemistry at the Interdisciplinary Center for Scientific Computing of Heidelberg University. His research interests comprise the development of electronic structure methods and their application in Photochemistry, Mechanochemistry, Biophysics, and Material Science.

Representative Publications:

1. D. R. Rehn, Z. Rinkevicius, M. F. Herbst, X. Li, M. Scheurer, M. Brand, A. L. Dempwolff, I. E. Brumboiu, T. Fransson, **A. Dreuw**, P. Norman, *WIREs Comput. Mol. Sci.* **2021**, *11*, e1528.
2. C. Slavov, C. Yang, A. H. Heindl, H. A. Wegner, **A. Dreuw**, J. Wachtveitl, *Angew. Chem. Int. Ed.* **2020**, *59*, 380.
3. S. Müller, J. Lüttig, P. Maly, L. Ji, J. Han. T. B. Marder, U. H. F. Bunz, **A. Dreuw**, C. Lambert, T. Brixner, *Nat. Comm.* **2019**, *10*, 1.
4. X. Yang, M. Hoffmann, F. Rominger, T. Kirschbaum, **A. Dreuw**, M. Mastalerz, *Angew. Chem. Int. Ed.* **2019**, *58*, 10650.
5. N. Alagna, J. Han, N. Wollscheid, J. L. Perez Lustres, J. Herz, S. Hahn, S. Koser, F. Paulus, U. H. F. Bunz, **A. Dreuw**, T. Buckup, M. Motzkus, *J. Am. Chem. Soc.* **2019**, *141*, 8834.
6. C. Slavov, C. Yang, A. H. Heindl, H. A. Wegner, **A. Dreuw**, J. Wachtveitl, *Angew. Chem. Int. Ed*. **2020**, *59*, 380**.**
7. H. Reiss, L. Ji, J. Han, S. Koser, O. Tverskoy, J. Freudenberg, F. Hinkel, M. Moos, A. Friedrich, I. Krummenacher, C. Lambert, H. Braunschweig, **A. Dreuw**, T. B. Marder, U. H. F. Bunz, *Angew. Chem. Int. Ed*. **2018**, *57*, 9543
8. P. Norman, **A. Dreuw**, *Chem. Rev.* **2018**, *118*, 7208
9. C. Yang, C. Slavov, H. A. Wegner, J. Wachtveitl, **A. Dreuw**, *Chem. Sci*. **2018**, *9*, 8665
10. J. Li, A. Friedrich, I. Krummenacher, A. Eichhorn, H. Braunschweig, M. Moos, S. Hahn, F. L. Geyer, O. Tverskoy, J. Han, C. Lambert, **A. Dreuw**, T. B. Marder, U. H. F. Bunz, *J. Am. Chem. Soc.* **2017**, *139*, 15968

Quasi-Particles in Chemistry

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Quasi-particles are not real particles, but many-body phenomena which behave like particles, and which can thus be described with particle theories, for example, excitons or plasmons. In this pedagogical talk, I will explain how these physics-inspired quasi-particles relate to quantum chemistry and chemical concepts. An exciton wavefunction will be derived from a many-body wavefunction and exciton properties calculated, which yield new insights into electronic structure of molecules but also into limitations of quantum chemical methods. Also, the question whether and how plasmons, the collective motion of many electrons, can be identified in molecules will be addressed.

References and Notes:

1. C. M. Krauter, S. Bernadotte, C. R. Jacob, M. Pernpointner and A. Dreuw *J. Phys. Chem. C* **2015**, *119*, 24564.
2. S. Bäppler, F. Plasser, M. Wormit and A. Dreuw *Phys. Rev. A* **2014**, *90*, 052521.

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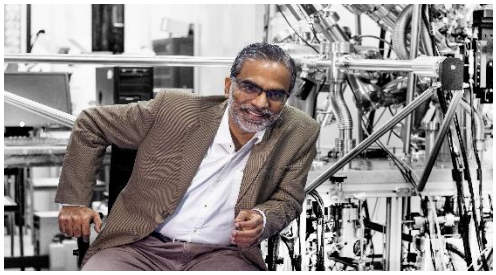

Prof. Thalappil Pradeep is an Institute Professor at the Indian Institute of Technology Madras, Chennai, India. He is the Deepak Parekh Institute Chair Professor and is also a Professor of Chemistry. He studied at the University of Calicut, Indian Institute of Science, UC Berkeley, and Purdue. His research interests are in molecular and nanoscale materials, and he develops instrumentation for such studies.

He is an author of over 525 scientific papers in journals and is an inventor of over 100 patents or patent applications. In addition to the work on advanced materials, he is involved in the development of affordable technologies for drinking water purification and some of them have been commercialized. His pesticide removal technology is estimated to have reached about 10 million people. Along with his associates, he has incubated seven companies and three of them have production units. His arsenic removal technology, approved for national implementation, is delivering arsenic free water to about 1.2 million people every day.

He is a recipient of several awards including the Shanti Swaroop Bhatnagar Prize, BM Birla Science Prize, National Award for Nanoscience and Nanotechnology, India Nanotech Innovation Award, JC Bose National Fellowship and National Water Award. He is the winner of The World Academy of Sciences (TWAS) prize in Chemistry for the year 2018. The nation conferred Padma Shri on him in 2020. He is also the recipient of Nikkei Asia Prize 2020. He has been named as a laureate of the 2022 Prince Sultan Bin Abdulaziz International Prize for Water. He is a Fellow of all the science and engineering academies of India, The World Academy of Sciences and American Association for the Advancement of Science. He is a distinguished professor in a few institutions in India and is also on the graduate faculty of Purdue University. He is the author of the introductory textbook, *Nano: The Essentials* (McGraw-Hill) and is one of the authors of the monograph, *Nanofluids* (Wiley-Interscience) and an advanced textbook, *A Textbook of Nanoscience and Nanotechnology* (McGraw-Hill). He is on the editorial boards of journals such as *ACS Nano*, *Chemistry of Materials*, *Analytical Chemistry*, *Chemical Communications*, *Chemistry – An Asian Journal*, *Nanoscale*, *Nanoscale Horizons*, *npj* Clean Water, etc., and is an associate editor of *ACS Sustainable Chemistry & Engineering.* He has authored popular science books in Malayalam and is the recipient of *Kerala Sahitya Akademi Award* for knowledge literature. He has received the *Lifetime Achievement Research Award* of IIT Madras and *Distinguished Alumnus Award* of IISc. As part of his philanthropic activities, he supports a school in his village where 500 students are on rolls.

Complexity in the Chemistry of Atomically Precise Clusters

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

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

References and Notes:

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7. Jana, P. Unnikrishnan, A. Poonia, J. Roy, M. Jash, G. Paramasivam, J. Machacek, K. N. V. D. Adarsh, T. Base, and T. Pradeep, *Inorg. Chem.* **2022**, *61*, 8593.

Prof. Dr. Alexander Heckel

Professor for Chemical Biology and Medicinal Chemistry

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1992-1997	Graduate Studies in Chemistry, University of Constance, Diplom, Thesis Supervisor: Prof. Dr. R. R. Schmidt
1997-2001	Ph.D. Thesis (Chemistry) with Prof. Dr. D. Seebach, ETH Zurich, Switzerland
2001-2003	Postdoc with Prof. Dr. P. B. Dervan, Caltech, USA
2003-2007	Liebig- and Emmy Noether-Junior Research Group Leader University of Bonn, Mentor: Prof. Dr. M. Famulok
2007-	Professor for Chemical Biology and Medicinal Chemistry Goethe-University Frankfurt

ORCID: 0000-0003-3541-4548 Researcher-ID: A-8498-2008

1. Solid-Phase-Supported Chemoenzymatic Synthesis of a Light-Activatable tRNA Derivative A. Blümler, H. Schwalbe,* A. Heckel,* *Angew. Chem. Int. Ed.* **2022**, *61*, e202111613, DOI: 10.1002/anie.202111613
2. Controlling Coagulation in Blood with Red Light“, P. Müller, M. Sahlbach, S. Gasper, G. Mayer,* J. Müller,* B. Pötzsch,* A. Heckel,* *Angew. Chem. Int. Ed.* **2021**, *60*, 22441-22446, DOI: 10.1002/anie.202108468
3. Differential Regulation of Local mRNA Dynamics and Translation Following Long-Term Potentiation and Depression, P. G. Donlin-Asp, C. Polisseni, R. Klimek, A. Heckel, E. M. Schuman,* *Proc. Natl. Acad. Sci. USA* **2021**, *118*, e2017578118, DOI: 10.1073/pnas.2017578118
4. Conformational Dynamics of Strand Register Shifts in DNA G-Quadruplexes“ J. T. Grün, C. Hennecker, D.-P. Klötzner, R. W. Harkness, I. Bessi, A. Heckel, A. K. Mittermaier,* H. Schwalbe,* *J. Am. Chem. Soc.* **2020**, *142*, 264–273, DOI: 10.1021/jacs.9b10367
5. A Light-Responsive RNA Aptamer for an Azobenzene Derivative“, T. S. Lotz, T. Halbritter, C. Kaiser, M. M. Rudolph, L. Kraus, F. Groher, S. Steinwand, J. Wachtveitl,* A. Heckel,* B. Suess,* *Nucleic Acids Res.* **2019**, *47*, 2029–2040, DOI: 10.1093/nar/gky1225
6. Chemo-Enzymatic Synthesis of Position-Specifically Modified RNA for Biophysical Studies including Light Control and NMR Spectroscopy, S. Keyhani, T. Goldau, A. Blümler, A. Heckel,* H. Schwalbe,* *Angew. Chem. Int. Ed.* **2018**, *57*, 12017–12021, DOI: 10.1002/anie.201807125
7. Life Times of Metastable States Guide Regulatory Signaling in Transcriptional Riboswitches C. Helmling, D.-P. Klötzner, F. Sochor, R. A. Mooney, A. Wacker, R. Landick, B. Fürtig, A. Heckel,* H. Schwalbe,* *Nat. Commun.* **2018**, *9*, 944, DOI: 10.1038/s41467-018-03375-w
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9. Activity-Dependent Spatially Localized miRNA Maturation in Neuronal Dendrites S. Sambandan, G. Akbalik, L. Kochen, J. Rinne, J. Kahlstatt, C. Glock, G. Tushev, B. Alvarez-Castelao, A. Heckel,* E. M. Schuman,* *Science* **2017**, *355*, 634–637, DOI: 10.1126/science.aaf8995
10. Light-Inducible AntimiR-92a as a Therapeutic Strategy to Promote Skin Repair in Healing-Impaired Diabetic Mice, T. Lucas, F. Schäfer, P. Müller, S. A. Eming, A. Heckel,* S. Dimmeler,* *Nat. Commun.* **2017**, *8*, 15162, DOI: 10.1038/ncomms15162.

Regulation of Oligonucleotides in Time and Space

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The past decades have taught us that RNA is exquisitely more than just a transitory carrier of genetic information. In the majority of these functions, in order to fulfil its role, aspects of RNA distribution in time and space play an important role. In order to address these questions, we developed tools that use light as external addressing signal for the spatio-temporal resolution. These tools allow for example the real-time tracking of RNA in three dimensions in a microscope.[1] Perfection of these methods allowed us to extend the detection time from minutes to up to 14 hours in neuronal tissue.[2] In further studies we could watch the local birth of a mature miRNA as response to local stimulation[3] or the live trafficking of RNA transport granules.[4] Importantly, using light as addressing scheme goes beyond watching all the way to active control.[5] We could just increase the versatility of this approach by the development of new chemo-enzymatic methods for the synthesis of modified RNA.[6]

References and Notes:

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Prof. Dr. Alakesh Bisai

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Alakesh obtained his Ph.D. from IIT Kanpur in Sept. 2006 in Asymmetric Catalysis with Prof. Vinod K. Singh. Immediately afterward, he moved to UC Berkeley, where he held postdoctoral position with Professor Richmond Sarpong (Sept. 2006 – Dec. 2009). During his stay at Berkeley, he completed the total synthesis of '*lycopodium alkaloids*' lyconadin A, that received considerable attention from the synthetic community. In Dec. 2009, he left Berkeley and joined Department of Chemistry, IISER Bhopal as an Assistant Professor of Chemistry, later he was promoted to an Associate Professor followed by Professor (Jan., 2018) and continued his Academic journey till May, 2020. He moved to the Department of Chemical Sciences, IISER Kolkata in May, 2019 and set a research lab. on the synthesis of Natural Product and analogues for Drug Discovery. 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*'. The research of the AB research group has been appreciated in various forms, to name a few notable ones:

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 (STAR-2020)
CRSI Young Scientist Award (2018)
Lead Lecture, Pfizer Symposium, IISc Bangalore (2016)
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)

Apart from his Academic activities, he served Institutes in various capacities, to name notable ones:
***IISER Kolkata**:* Member, **IIC** (Institute Innovation Council) (Jan. 2020 – Dec. 2021); Member, **CMOS** [Campus Maintenance & Oversight Committee (Jan., 2022 –)]; Member, **Senate** (Academic) (May 20, 2019 – till date); Coordinator, **SRP** [Summer Research Program] (2020) for J & K and Ladakh (2022); Convener, **PGAC**, DCS (Jan. 2022 –); Convener, **Safety**, DCS (July 2019 – April, 2022); Member, **UGAC**, DCS (Jan. 2020 – Jan. 2022); Member, DCS Course Allocation Committee (DCAC) (Jan., 2020 - Dec., 2021); Expert Member, SERB-SIRE (2022 -), SERB-EMEQ (2022 -)
***IISER Bhopal**:* Chief Vigilance Officer (**CVO**) (Jul., 2015 – May, 2019); Dean of the Faculty Affairs (**DoFA**) (Jan., 2015 – Dec., 2016); Coordinator, **Outreach** Activities (Jan. 2015 – Dec. 2015); Member, Departmental Faculty Advisory Committee (**DFAC**) (Jan., 2013 - Dec., 2013 & Jan., 2017 – Dec., 2018); Member, Departmental Course Allocation Committee (**DCAC**) (Feb., 2017 - Dec., 2018); Member, **Senate** (Academic) (Jan., 2015 - May., 2020); Chairperson, Health Center User Committee (**HCUC**) (Jan., 2015 - Dec, 2016); Convener, **DUGC** and **DPGC**, Chemistry (Feb., 2011- Apr., 2013); Convener, Rate Contract Committee (Jan., 2011 - Dec., 2013); Member, Anti-Ragging Committee (July, 2010 - Dec., 2011)

Nature Inspired Oxidative Strategies for Dixiamycins & Taiwaniadducts

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Nature produces a variety of complex natural products in entioenriched form (see, Figure).[1-2] Since these are isolated from Nature in limited quantity (mostly in mg scale), total synthesis endeavors can play a crucial role in bioactivity evaluation by providing access to significant quantity.[1-4] It also provides platform for the innovation of new strategies for chemical synthesis.[5-6] In this regard, naturally occurring alkaloids with impressive diversity of biological activities drew our interest.[1a]

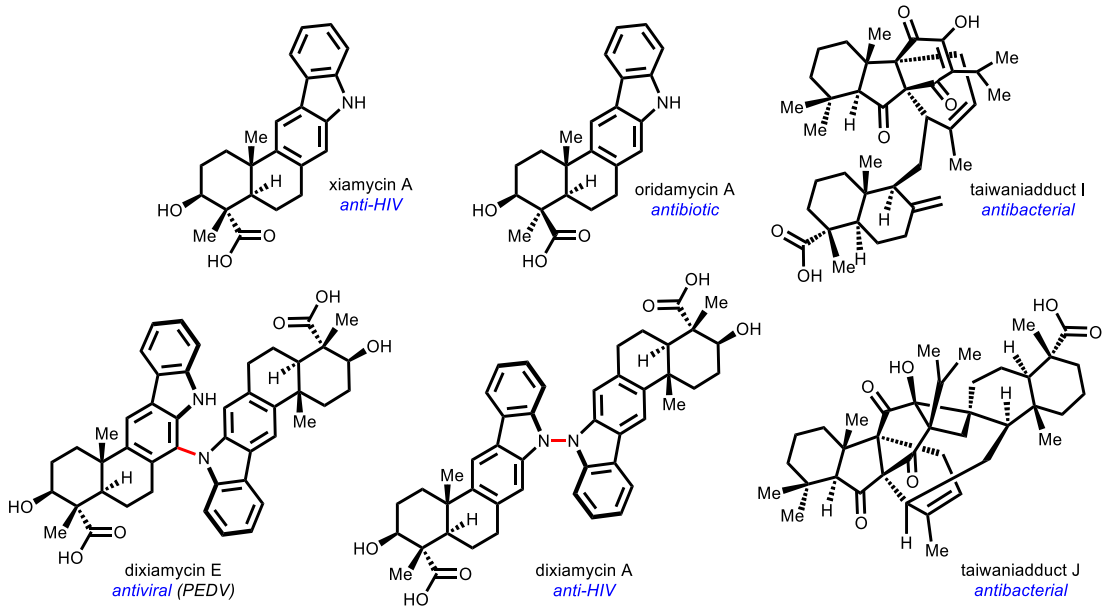

Figure. Architecturally intriguing indole alkaloids of biological relevance.

Interestingly, a variety of alkaloids of this family show interesting biological activities, such as antibacterial and cytotoxic activities.[1a] Towards this direction, we explored novel oxidative strategies under mild condition that will be discussed in this talk.[7]

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Career Profile

2019-present W2 Professor, Institute of Physical Chemistry, Goethe University Frankfurt, Germany
2013-2019 W1 Professor, Institute of Physical Chemistry, Goethe University Frankfurt, Germany
2011-2013 Senior Research Associate, University of Oxford, UK
2010-2011 Postdoctoral Research Associate, University of Oxford, UK, with Prof. Carol Robinson.
2008-2010 Postdoctoral Research Assistant, University of Cambridge, UK, with Prof. Carol Robinson.

Awards/achievements

2019 Heisenberg Professorship
2013 ERC Starting Grant

Representative publications

Vu Huu *et al*. Nature Communications | (2022)13:1218 | https://doi.org/10.1038/s41467-022-28828-1

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Biomolecular complexes: required and unwanted assemblies – what can we learn with native mass spectrometry?

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Assembly processes play an important role in the cellular environment. Large macromolecular complexes such as the ATPase from the respiratory chain, need to self-assemble into the correct complex structure in order to be fully functional. Opposed to these well guided processes there are assembly processes, which lead to less wanted structures, such as Amyloid-ß fibrils, which are correlated to Alzheimer's disease.

We investigate such processes by means of native mass spectrometry and ion mobility. We can reveal underlying mechanisms for the above mentioned processes, including environmental conditions which are prerequisite for assembly of the ATPase into a functional complex[1], or the weak point in the Amyloid-ß assembly[2], which allows to disrupt this process.

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2. Tobias Lieblein*, Rene Zangl*, Janosch Martin, Jan Hoffmann, Marie J Hutchison, Tina Stark, Elke Stirnal, Thomas Schrader, Harald Schwalbe, Nina Morgner, Structural rearrangement of amyloid-β upon inhibitor binding suppresses formation of Alzheimer disease related oligomers eLife 2020;9:e59306 https://doi.org/10.7554/eLife.59306

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Beeraiah Baire is from Choppadandi, Karimnagar of Telangana state. His initial schooling was done in Choppadandi. He obtained his B.Sc. from SRR Govt degree college, affiliated to Kakatiya University. He completed his M.Sc. (Chemistry) from the University of Hyderabad in 2003. He obtained his Ph.D. in Organic Chemistry, from IISc, Bangalore, with (Late) Prof. Srikrishna in Nov 2007. Later he moved to University of Minnesota for his postdoctoral studies where he worked with Prof. Thomas R Hoye, from Dec 2009 (Dec)- 2013 (Aug). In September 2013, he joined Department of Chemistry, IIT Madras as Assistant Professor. Currently, he is working as an Associate Professor in the same department.

His Research interests:

- ✓ Development of new synthetic strategies employing propargylic alcohols and derivatives as building blocks
- ✓ Total synthesis of Natural products

Key Research developments:

i) The Z-enoate assisted Meyer-Schuster Rearrangement
ii) A new *semi*-Favorskii rearrangement
iii) The Hexadehydro Diels-Alder (HDDA) reaction for benzyne generation and reactions (during Postdoctoral research)

Research Publications: 72; Patents: 1; Book chapters :2
PhD students: Graduated: 5; current: 8

The Z-enaote assisted Meyer-Schuster rearrangement: An umpolung functionalization of propargylic alcohols

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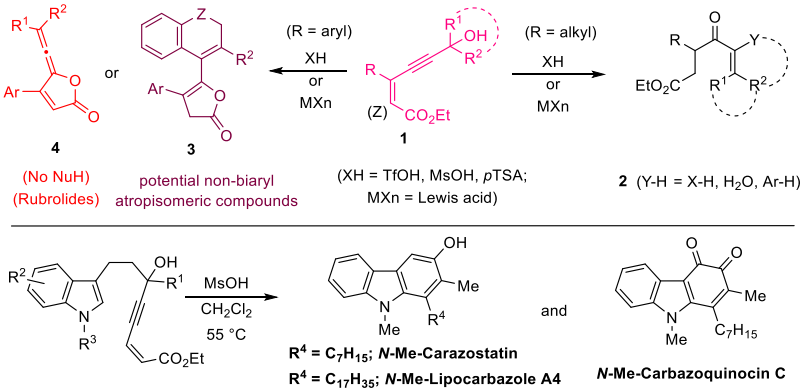
Propargylic alcohols and their derivatives are one of the most useful building blocks with two functional groups. These units have been employed in numerous cascade synthetic transformations in organic chemistry providing an opportunity to discover novel cascade processes.[1] In our laboratory we design and develop novel strategies based on acid catalysis employing propargylic alcohol derivatives as building blocks. Meyer–Schuster rearrangement is a widely utilized transformation involving an acid promoted 1,3-transposition of propargylic alcohols to α,β-enones.[2] Recently, our group has developed an umpolung strategy using Z-enoate propargylic alcohols[3] that allows nucleophilic interception of the proposed allenol intermediate of Meyer–Schuster rearrangement. The details of some of our latest discoveries and developments in this area will be discussed in the presentation.

Scheme: The Z-enaote assisted Meyer-Schuster rearrangement and developments



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