

**Indo-German Workshop-2022:
Complex Chemical Systems
(IGW-CCS-2022)**

OCTOBER 6-9, 2022

**Taj Fisherman's Cove Beach Resort
Mahabalipuram
India**

**Indo-German Workshop-2022: Complex Chemical Systems
(IGW-CCS-2022; 6-9 October 2022)**

Day-1: October 6, 2022 (Thursday)

Venue: Hotel Taj Fisherman's Cove, Mahabalipuram

Inauguration (3.00 – 3.15 PM)	<p>Welcome: G. Sekar (IIT Madras) Alexander Heckel (Goethe University-Frankfurt)</p> <p>Indo-German S&T Initiatives: Srivari Chandrasekhar (Secretary, DST)</p>
SESSION 1 (3.15 – 4.45 PM)	Chairperson: V. K. Singh (IIT Kanpur)
3.15 – 3.45 PM	Petra Tegeder (University of Heidelberg) <i>Electronic Properties of Interfaces with N-Heteropolycyclic Molecules</i>
3.45 – 4.15 PM	R. Mahalakshmi (IISER Bhopal) <i>Physico-chemical self-assembly landscape of the human voltage-gated anion channel</i>
4.15 – 4.45 PM	Anand Singh (IIT Kanpur) <i>Visible Light Mediated Functionalization of π-Systems</i>
4.45 – 5.15 PM	TEA / COFFEE BREAK
SESSION 2 (5.15 – 7.15 PM)	Chairperson: K. P. Kaliappan (IIT Bombay)
5.15 – 5.45 PM	Jürgen Seibel (University of Würzburg) <i>Sphingolipids in infection</i>
5.45 – 6.15 PM	N. D. Pradeep Singh (IIT Kharagpur) <i>Temporal Release of Cell Cycle Regulator α-lipoic acid: NIR-light Activatable Quinoxaline Based Nano-prodrug Delivery System</i>
6.15 – 6.45 PM	Jürgen Köhler (University of Bayreuth) <i>The light harvesting complex of the marine alga <i>Codium fragile</i>. Spectroscopy of single <i>siphonaxanthin</i>-<i>siphonein</i>-Chl-<i>a/b</i>-proteins (SCP): A Status Report</i>
6.45 – 7.15 PM	R. Madhan (Director, IGSTC) <i>Indo-German Science & Technology Centre (IGSTC)</i>
7.30 PM	MIXER & DINNER

Day-2; October 7, 2022 (Friday)

SESSION 3 (9.30 – 11.30 AM)	Chairperson: G. Mugesh (IISc Bangalore)
9.30 – 10.00 AM	Snorri Sigurdsson (University of Iceland) <i>Improving the sensitivity of NMR spectroscopy with stable radicals</i>
10.00 – 10.30 AM	Ramesh L. Gardas (IIT Madras) <i>Benign Solvents as Performance Additives to Enhance the Extraction of Micropollutants and Heavy metals</i>
10.30 – 11.00 AM	Josef Wachtveitl (Goethe-University Frankfurt) <i>Azobenzene photoswitch scaffolds: scope and (bio-)molecular applications</i>
11.00 – 11.30 AM	K. Geetharani (IISc Bangalore) <i>Development of N-Heterocyclic Carbene Complexes of Cobalt for Carbon-Boron Bond Formation</i>
11.30 – 12:00 Noon	TEA / COFFEE BREAK
SESSION 4 (12.00 – 1.30 PM)	Chairperson: Kausik Panda (Syngenta)
12:00 – 12.30 PM	Tomáš Slanina (IOCB Prague) <i>Reversibility in Photochemistry: Beyond the Classical Approaches</i>
12.30 – 1.00 PM	Dibyendu Das (IISER Kolkata) <i>Living Matter Like Materials via Complex Chemical Systems</i>
1.00 – 1.30 PM	Surajit Ghosh (IIT Jodhpur) <i>Engineered Antimitotic Peptide Evolved from Hotspots of Tubulin Interface</i>
1.30 – 2.30 PM	LUNCH
SESSION 5 2.30 – 4.30 PM	Chairperson: Snorri Sigurdsson (University of Iceland)
2:30 – 3.00 PM	Bernd Engels (University of Würzburg) <i>Boron Chemistry What Can Theory Contribute New And What To Pay Attention To For Accurate Calculations</i>
3.00 – 3.30 PM	Ravi P. Singh (IIT Delhi) <i>Dehydrogenative C-C and C-P Bond Formation</i>
3.30 – 4.00 PM	Andreas Dreuw (University of Heidelberg) <i>Quasi-Particles in Chemistry</i>
4.00 – 4.30 PM	P. Rajamalli (IISc Bangalore) <i>Organic Thermally Activated Delayed Fluorescence Emitters for Organic Light Emitting Diodes</i>
4.30 – 6.30 PM	TEA / COFFEE BREAK FREE TIME
6.30 – 7.30 PM	Panel Discussion: Sharing knowledge through open science and open access Moderator: V. K. Singh (IIT Kanpur) Sandeep Verma (IIT Kanpur/SERB), Alexander Heckel (Goethe University-Frankfurt), Ajit Sharma (RSC), Harshita Pawar (ACS) and Khushbu Kushwaha (Wiley-VCH)
7.30 PM	BANQUET DINNER

Day-3: October 8, 2022 (Saturday)

SESSION 6 (9.30 – 11.00 AM)	Chairperson: H. N. Ghosh (BARC Bombay)
9.30 – 10.00 AM	Nina Morgner (Goethe-University Frankfurt) <i>Biomolecular complexes: required and unwanted assemblies – what can we learn with native mass spectrometry?</i>
10.00 – 10.30 AM	Prasanta K. Das (IACS, Kolkata) <i>Organic Nanostructures in Cellular Transportation</i>
10.30 – 11.00 AM	Nidhi Gour (Indrashil University) <i>Metabolite amyloids and its possible implications in disease etiology</i>
11.00 – 11.30 AM	TEA / COFFEE BREAK
SESSION 7 (11.30 – 1.00 PM)	Chairperson: Bernd Engels (University of Würzburg)
11.30 – 12.00 noon	Alexander Heckel (Goethe-University Frankfurt) <i>Regulation of Oligonucleotides in Time and Space</i>
12.00 – 12.30 PM	S. G. Srivatsan (IISER Pune) <i>Probing nucleic acid conformations using responsive nucleoside probes</i>
12.30 – 1.00 PM	T. Govindaraju (JNCASR, Bangalore) <i>Molecular Theranostics</i>
1.00 – 1.10 PM	Concluding Remarks Sandeep Verma (IIT Kanpur/SERB) Closure of IGW-CCS-2022
1.10 – 2.00 PM	LUNCH
2.00 – 6.30 PM	Excursion to Mahabalipuram
7.30 PM	DINNER

October 9, 2022 (Sunday)

Departures After Breakfast

**Chairpersons / Panel Members /
Special Invitees**

Vinod K. Singh

Professor

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Professor Vinod Singh is currently Rahul and Namita Gautam Chair Professor in the Department of Chemistry at IIT Kanpur. He also holds Director's Chair Professor at IISER Bhopal. He is currently the President, the Chemical Research Society of India (CRSI) and the Chairperson of the Governing Council of IACS Kolkata.

Professor Singh did Ph.D. under the guidance of Dr Sukh Dev from Multi-Chem Research Center, Nandesari, Baroda (M.S. University, 1986). He spent 2 years of 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, he joined IIT Kanpur in 1990 as an Assistant Professor and rose to the rank of Professor.

He works in the area of synthetic organic chemistry, especially asymmetric synthesis. His research work 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 all the science academies of the country and The World Academy of Sciences (FTWAS).

He is an Editor of an Elsevier journal - Tetrahedron Lett. He is a Member of, the Editorial Advisory Board of Org. Lett., J. Org. Chem., Asian J. Org. Chem., and Org. Chem. Frontiers.

As a Founding Director of IISER Bhopal for more than 10 years (2008-2018), Professor Singh built the Institution 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.

In 2020, he was given TWAS-CASAREP award for building a scientific institution. He had been a Member of the Scientific Advisory Council to the Prime Minister (SAC to PM) during 2009-2014.

S. Chandrasekhar

Secretary, DST

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Asian Scientist Magazine (Jul. 5, 2016) published an article on 8 Scientists From India To Watch Wherein they featured a handful of Indian scientists that are breaking new ground in space, biomedical science, pharmaceuticals and beyond. Dr. Chandrasekhar was one amongst them along with Bharat Ratna Prof. CNR Rao, Kiran Majumdar Shaw etc.

- Dr. Srivari Chandrasekhar has made significant contributions in diverse areas of organic chemistry especially in chiral chemistry and total synthesis of biologically active natural products (marine natural products with architectural complexity).
- The development of PEG as a novel solvent medium created a totally different platform for practitioners of Green chemistry.
- Development of new methodologies for C-C bond formation reactions involving organo-catalysis and organo-metallic reagents is highly cited.
- Process development and drug discovery in collaboration with pharmaceutical industry have resulted in development of economically viable processes and lead compounds.
- He has 300 publications and 22 patents with over 7000 citations.
- 80 students have already obtained their Ph.D. award under his able guidance and 20 students are currently pursuing their research work with Dr. S. Chandrasekhar.
- He was awarded A V Rama Rao Chair in 2020
- His team was awarded CSIR Technology Award 2021 for the process for vaccine adjuvant in Covaxin, 2020, for the process of Favipiravir and 2014 for the process of Misoprostol in 2014.
- He received the Golden Jubilee Commemoration Medal (Chemical Sciences 2020) from INSA.
- He has been honoured by Chemical Research Society of India (CRSI) by CRSI Silver Medal for his extensive and outstanding contributions to research in Chemistry.
- He has been selected for the Astra Zeneca Research Endowment Award for the year 2019.
- He is recipient of Infosys Prize 2014 for Physical Sciences, CNR Rao National Prize in Chemical Research 2012, SASTRA-CNR Rao award for excellence in Material and Chemistry in 2017, Goyal Prize in Chemical Sciences 2017 and VASVIK Award 2018 for Chemical Sciences and Technology.
- He received Sir C V Raman Birth Centenary Award for 2018.
- He is a recipient of the National Academy of Sciences-Reliance platinum jubilee award in physical sciences for work on innovations in applied research with fundamental approach.
- He has been awarded the Ranbaxy Research award in Pharmaceutical Sciences-2009 for his contributions to total synthesis of natural products and medicinal chemistry.
- He is a fellow of the Indian Academy of Sciences, Indian National Science Academy and National Academy of Sciences.
- Dr. Srivari obtained his Bachelors, Masters and Ph. D. degree from Osmania University while the work for Ph. D. was carried out in IICT on total synthesis of Cyclosporin.
- He was Alexander von Humboldt Fellow at Goettingen and post-doctoral fellow at University of Texas.

Sandeep Verma

Professor

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Prof. Sandeep Verma has been associated with IIT Kanpur since 1997 and he currently serves as the Secretary, Science and Engineering Research Board. His research interests include chemical neuroscience, stem cell engineering, and new antibiotics. With over 200 publications and several patents to his credit, his work has been recognized by Shanti Swarup Bhatnagar Prize, Distinguished Alumnus Award of Banaras Hindu University, Goyal Prize in Chemical Sciences, and Swarnajayanti Fellowship, to name a few. He is an elected *Fellow* of all major academies of science and engineering: Indian National Science Academy, Indian Academy of Sciences, National Academy of Sciences, and Indian National Academy of Engineering. He is an Associate Editor of *Chemical Communications* (RSC, UK) and serves on the Editorial Advisory Board of *ChemBioChem* (Wiley).

G. Mugesh

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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. 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.

G. Mugesh received several awards and recognitions, which include: Distinguished Alumnus Award of IIT Bombay for the year 2021; SASTRA-CNR Rao Award in Chemistry & Materials Science for the year 2021; Infosys Prize in Physical Sciences by Infosys Science Foundation; CRSI Silver Medal, Chemical Research Society of India; National Prize for Research on Interfaces of Chemistry and Biology by C. N. R. Rao Education Foundation and AVRA Laboratories Pvt. Ltd.; J. C. Bose National Fellowship, DST-SERB, Government of India; Shanti Swarup Bhatnagar Prize for the year 2012; AstraZeneca Excellence in Chemistry Award; Swarnajayanti Fellowship for 2006-7. He is a fellow of the National Academy of Sciences, India (NASI), Indian Academy of Sciences (IAS), Indian National Science Academy (INSA) and the Royal Society of Chemistry (RSC).

Representative Publications:

1. Singh, N.; NaveenKumar, S. K.; Geethika, M.; Mugesh, G. Cerium vanadate nanozyme with specific superoxide dismutase activity regulates mitochondrial function and ATP synthesis in neuronal cells. *Angew. Chem. Int. Ed.* **2021**, *60*, 3121 - 3130.
2. Chakrabarty, G.; NaveenKumar, S. K.; Kumar, S.; Mugesh, G. Modulation of Redox Signalling and Thiol Homeostasis in Red Blood Cells by Peroxiredoxin Mimetics. *ACS Chem. Biol.* **2020**, *15*, 2673 – 2682.
3. Ungati, H.; Govindaraj, V.; Narayanan, M.; Mugesh, G. Probing the formation of a Seleninic Acid in Living Cells by a Fluorescence Switching of a Glutathione Peroxidase Mimetic. *Angew. Chem. Int. Ed.* **2019**, *58*, 8156 - 8160.
4. Jakka, S.R.; Govindaraj, V.; Mugesh, G. A Single Atom Change Facilitates the Membrane Transport of Green Fluorescent Proteins in Mammalian Cells. *Angew. Chem. Int. Ed.* **2019**, *58*, 7713 - 7717.

Krishna P. Kaliappan

Dean Strategy & Professor of Chemistry

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Krishna P. Kaliappan, after his Ph.D from Indian Institute of Science, Bangalore, spent two years each at University of Geneva (97-98) and at Duke University (99-00) for his post-doctoral studies before joining IIT Bombay as an Assistant Professor in 2001. He became full Professor in 2009 and Institute Chair Professor during 2014-2020. He has been a Visiting Professor at University of Massachusetts, Amherst and at ESPCI, Paris. He served as Associate Dean (R & D) at IIT Bombay (2012-2015), Head of Chemistry Department (2016-2018) and Dean (Faculty Affairs) (2018-2021). He is currently Dean Strategy of Indian Institute of Technology Bombay. He has been on the Editorial Advisory Board of Chemistry An Asian Journal Chemistry (2014-2021) and on the Editorial Advisory Board of Organic and Biomolecular Chemistry Journal (2014-2021). He is a Fellow of the Royal Society of Chemistry (FRSC) since 2008 and Fellow of Indian Academy of Sciences, Bangalore (FASc) since 2016. He has been a member of the sub-committee of IUPAC Organic and Biomolecular Division since 2015. He was the Organizing Chairman of ICOS 21 (21st International Conference on Organic Synthesis). He has received Prof. C. N. R. Rao National Prize in Chemical Sciences, Swarnajayanti Fellowship and B. M. Birla prize in recognition of his research contribution. He has also received Prof. S. C. Bhattacharyya award for excellence in research (in pure sciences), excellence in Teaching award and best research paper award from IIT Bombay. His current research interests include total synthesis of natural products, domino strategy to synthesis of complex natural products and natural product like molecules. He has guided 25 Ph.D students and supervising currently 15 Ph.D students.

Hirendra N. Ghosh

Designation: Scientific Officer (H)

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Awards/Recognition

Fellow of Indian National Science Academy (FNA), New Delhi
Fellow of Academy of Science (FASc), Bangalore,
Fellow of National Academy of Science (FNASc), Allahabad
CRSI Silver Medal
DAE-SRC Outstanding Investigator Award
Homi Bhabha Science & Technology Award
J. C. Bose National Fellow

Representative publications

ACS Photonics **2022**, *9*, 969-978.
ACS Photonics **2022**, *9*, 2756-2766.
J. Phys. Chem. Letters **2022**, *13*, 83–90.
J. Phys. Chem. Letters **2021**, *12*, 11865–11872.
J. Phys. Chem. Letters **2021**, *12*, 6526–6534.
J. Phys. Chem. Letters **2021**, *12*, 5000–5008.
J. Phys. Chem. Letters **2021**, *12*, 10958–10968.

Harshita Pawar

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Career Profile:

Dr. Harshita Pawar is working as a Development Editor with the American Chemical Society. She is responsible for facilitating the Development Editor workflow and streamlining the editorial decision-making process with the goal of creating and maintaining a positive author experience. She obtained her doctoral degree in Atmospheric Sciences from the Indian Institute of Science Education and Research (IISER) Mohali. Before her doctoral research, she completed an Integrated BS-MS from IISER Mohali with Chemistry as her major.

Representative publications:

1. Pawar, H., et al. "Quantifying the contribution of long-range transport to particulate matter (PM) mass loadings at a suburban site in the north-western Indo-Gangetic Plain (NW-IGP)." *Atmospheric Chemistry and Physics* 15.16 (2015): 9501-9520.
2. Pawar, Harshita, and Baerbel Sinha. "Humidity, density, and inlet aspiration efficiency correction improve accuracy of a low-cost sensor during field calibration at a suburban site in the North-Western Indo-Gangetic plain (NW-IGP)." *Aerosol Science and Technology* 54.6 (2020): 685-703.

Kausik Panda

Senior Team Leader

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Short Career Profile:

Currently working as *Senior Team Leader*, Research & Technology, Syngenta Biosciences Pvt Ltd, Goa, India.

Completed *Ph. D.* from I.I.T. Kanpur, India (2004) under supervision of Prof. H. Ila. followed by *Postdoctoral research* in Department of Medicinal Chemistry, University of Kansas, USA. Joined GVK Biosciences Pvt. Ltd., Hyderabad, India in 2007 as *Senior Scientist* in *Medicinal Chemistry Division*. After that joined EVOTEC (India) Ltd., Mumbai, India (2008) as *Group Leader*. Then worked as *Senior Principal Investigator (Synthetic & Med Chem division)* in 2010 in SYNGENE International Ltd. (A Biocon Company) Bangalore, India. Prior to Syngenta, was working as *Director (GM)*, and *Head (Chemical Profile Group)*, I&DC-API, FRESSENIUS KABI ONCOLOGY Ltd., Gurgaon, India, till July 2022.

Significant awards/achievements: NIH Fellowship (USA), JRF-SRF-RA (CSIR), GATE. Actively participated in various symposium/conferences nationally & internationally hosted by NIH / ACS / ISCB / CRSI etc

Publications in Journals of ACS, *Thieme*, Elsevier, Wiley-VCH etc and US-patent with Merck KgGA GmbH, Germany.

Ajit Sharma

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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.

Khushbu Kushwaha

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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 portfolio of *Chemistry Europe* and *ACES* journals as an acquisition editor at conferences and workshops.

Invited Lectures

Petra Tegeder

Professor

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|-----------------|--|
| 2021 | Offer for a professorship (W3) in Physical Chemistry at the Christian-Albrechts-Universität zu Kiel (declined) |
| 2018 | Offer for a professorship (W3) in Interfacial Analytics at the Freie Universität Berlin (declined) |
| Since 11/2012 | University Professor (W3) for Physical Chemistry, Ruprecht-Karls-Universität Heidelberg |
| 08/2010-10/2012 | University Professor (W2) for Experimental Physics, Freie Universität Berlin |
| 07/2004-07/2010 | Senior Research Scientist (C1), Institut für Experimentalphysik, Freie Universität Berlin with Prof. M. Wolf |
| 10/2004 | Visiting Scientist (DAAD), University of Minnesota (USA) with Prof X.Y. Zhu |
| 03/2002-06/2004 | Research Associate, Institut für Experimentalphysik, Freie Universität Berlin with Prof. M. Wolf |
| 03/2000-02/2002 | Marie Curie Postdoctoral fellow at the University College London, Department of Physics and Astronomy with Prof. N. J. Mason |
| 01/2000 | Visiting Scientist (DAAD) at the Tata Institute of Fundamental Research (Mumbai, India) with Prof. E. Krishnakumar |
| 12/1999 | PhD in Chemistry, Physical Chemistry, Freie Universität Berlin, with Prof. E. Illenberger |
| 04/1996 | Diploma in Chemistry, Freie Universität Berlin |

Electronic Properties of Interfaces with N-Heteropolycyclic Molecules

Petra Tegeder

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For improvement and optimization of the performance of organic molecule-based devices, such as photovoltaic cells and thin-film transistors comprehensive insight into the physical and chemical properties of the organic molecules at surfaces is necessary.

N-heteropolycyclic aromatic compounds are promising candidates for n-channel semiconductors. The introduction of nitrogen atoms into the π -backbone of the polycyclic aromatic hydrocarbons stabilizes the frontier orbitals and increases the electron affinity, while the size of the HOMO-LUMO (optical) gap is nearly unaffected. By using two-photon photoemission spectroscopy (2PPE) and high resolution electron energy loss spectroscopy (HREELS) we determined quantitatively transport, singlet and triplet states as well as electronic spectra of several N-heteropolycyclic molecules adsorbed on Au(111) [1-4]. Using angle-resolved 2PPE we identified strongly dispersing occupied and unoccupied electronic states, which result from hybridization between localized molecular states and delocalized metal bands at the metal/organic interface [2, 3].

We acknowledge funding by the German Research Foundation through the SFB 1249 (N-Heteropolycycles as Functional Materials) and the Cluster of Excellence (3D Matter Made to Order).

References

1. M. Ajdari, T. Schmitt, M. Hoffmann, F. Maaß, H. Reiss, U. H. F. Bunz, A. Dreuw, P. Tegeder, *J. Phys. Chem. C* **124** (2020) 13196.
2. A. Stein, D. Rolf, C. Lotze, B. Günther, L. H. Gade, K. J. Franke, P. Tegeder, *J. Phys. Chem. Lett.* **12** (2021) 947.
3. A. Stein, D. Rolf, C. Lotze, S. Feldmann, D. Gerbert, B. Günther, A. Jeindl, J.J. Cartus, O.T. Hofmann, L.H. Gade, K.J. Franke, P. Tegeder, *J. Phys. Chem. C* **125** (2021) 19969.
4. M. Hoffman, M. Ajdari, F. Landwehr, O. Tverskoy, U. H. F. Bunz, A. Dreuw, P. Tegeder, *Phys. Chem. Chem. Phys.*, **24** (2022) 3924.

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Career Profile

Prof. R. Mahalakshmi studies the folding, function, and regulation of the human mitochondrial metabolite flux protein VDAC, the core translocase protein Tom40, and the mitochondrial outer membrane chaperone Sam50 as well as its bacterial homolog BamA. She uses biophysical tools, spectroscopic techniques, and single molecule ensemble studies to characterize membrane proteins at the molecular level. The overarching goal of Mahalakshmi's research is to develop feasible translational strategies targeted at cancer, neurodegeneration, and bacterial infections using membrane proteins.

Notable awards and recognitions (2017-2022)

Featured in the DST Coffee Table Book "75 under 50 Scientists Shaping Today's India", a compendium published by Vigyan Prasar (2022).
Elected as Fellow of the National Academy of Sciences, India (NASI) (2021).
DBT – Wellcome Trust India Alliance Senior Fellowship (2020).
SwarnaJayanti Fellowship, Department of Science and Technology, Govt. of India (2020).
Young Researcher Award, Lady Tata Memorial Trust (2019).
Young Scientist Award, Indian Peptide Society (2019).
SERB Women Excellence Award (2017).

Representative recent publications

George, A, Ravi, R, Tiwari, PB, Srivastava, SR, Jain, V and **Mahalakshmi, R***. Engineering a Hyperstable *Yersinia pestis* Outer Membrane Protein Ail Using Thermodynamic Design. **J. Am. Chem. Soc.** **2022**, 144(4):1545-1555 (DOI: 10.1021/jacs.1c05964).

Tiwari, PB and **Mahalakshmi, R***. Interplay of protein primary sequence, lipid membrane, and chaperone in β -barrel assembly. **Protein Sci.** **2021**, 30(3):624-637 (DOI: 10.1002/pro.4022).

Srivastava, SR and **Mahalakshmi, R***. Evolutionary selection of a 19-stranded mitochondrial β -barrel scaffold bears structural and functional significance. **J. Biol. Chem.** **2020**, 295(43):14653-14665 (DOI: 10.1074/jbc.RA120.014366).

Iyer, BR and **Mahalakshmi, R***. Hydrophobic characteristic is energetically preferred for cysteine in a model membrane protein. **Biophys. J.** **2019**, 117:25-35 (DOI: 10.1016/j.bpj.2019.05.024).

Physico-chemical self-assembly landscape of the human voltage-gated anion channel

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Human voltage-dependent anion channels (VDACs) are vital 19-stranded β -barrel metabolite transporters of the mitochondrial outer membrane. Unlike the pro-apoptotic VDAC1, the human VDAC2 isoform is particularly of pharmacological interest due to its anti-apoptotic nature. In addition to ATP/ADP and NADH flux, as well as calcium homeostasis, VDAC2 is selectively upregulated in cancer. Yet, we know strikingly little about the molecular regulators of VDAC2 structure, voltage-dependent gating, and functional bioenergetics. Here, we carry out a comprehensive characterization of the folding pathway of human VDAC2 in phosphocholine membranes. We show that early events in the assembly of the 19-stranded structure involves parallel pathways. The kinetically faster pathway, although more populated, shows the rapid accumulation of an off-pathway intermediate that subsequently undergoes slow rearrangement to the native VDAC2 structure. The slow folding intermediate forms non-native contacts in both the lumen- and lipid-facing residues throughout the primary sequence. Interestingly, residues of the C-terminal strands β 15– β 19 form non-native interactions in both pathways, allowing us to link our findings with the chaperone-assisted *in vivo* assembly of VDAC2. Once folded, the VDAC2 β -barrel is trapped in an energetically compromised structure, with charged residues of the intrinsically destabilized strands β 2– β 7 essential to regulate voltage-gated channel opening, ATP flux, and *in vivo* survival. Noteworthy here is how residues of these N-terminal strands, vital both for overcoming the transition state barrier during barrel assembly and VDAC2 function, inversely regulate its thermodynamic stability. In contrast, although the C-terminal strands β 15– β 19 affect VDAC2 folding, they function as post-folding anchors in the membrane. A zonal inter-regulation of folding, stability, and function we see in VDAC2 also accounts for the evolutionary demarcation of both isoforms in the mitochondrial outer membrane.

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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.

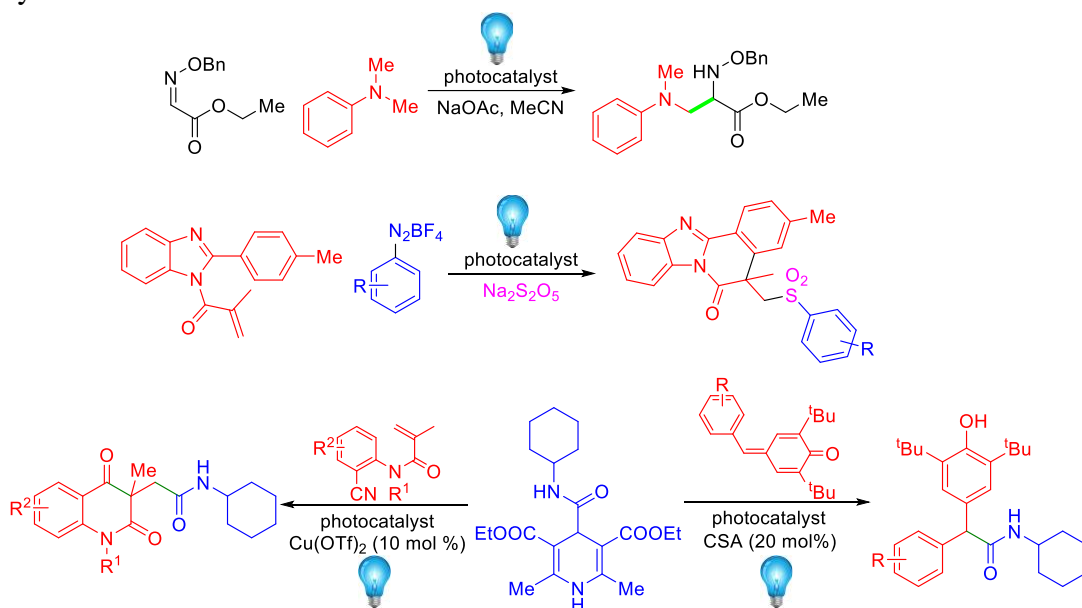
Visible Light Mediated Functionalization of π -Systems

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The generation of molecular diversity and complexity in short order remains the overarching goal of new synthetic strategies. The success and popularity of such methods are primarily driven by the advantage of being able to employ readily available and minimally functionalized starting materials. As a corollary, an enormous amount of new chemical space can be potentially created in an efficient manner. Our laboratory has been working on the expeditious functionalization of various π -systems for the development of new routes toward heterocycles and fluorinated molecules. The activation of diverse small molecule precursors and their reactions with olefins¹, allenes² and arynes³ encompass a versatile reactivity platform. The development of new methods involving visible light promoted activation of small molecule synthons will be discussed.



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- Garg, P; Singh, A.* "Unmasking Dipole Character of Acyl Ketene Dithioacetals via A Cascade Reaction with Arynes: Synthesis of Benzo[b]thiophenes" *Org. Lett.* **2018**, 20, 1320.

JÜRGEN SEIBEL

Professor

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Academic career

- 04/09 Professor (W2) of Organic Chemistry, University of Würzburg
- 05/07 – 03/09 Group Leader at Helmholtz Centre for Infection Biology, Stöckheim
- 12/06 Venia legendi, Habilitation in Bioorganic Chemistry, TU Braunschweig
- 07/02 – 12/06 Research Assistant (C1) Department of Chemistry, University of Braunschweig
- 08/00 – 06/02 Postdoctoral Fellow with Prof. Chris J. Schofield, The Department of Chemistry, The Dyson Perrins Laboratory, University of Oxford
- 11/97 – 07/00 Ph.D studies at the Institute of Organic Chemistry, University of Göttingen under the supervision of Prof. Dr. Dr. h.c. L.F. Tietze
- 10/92 – 10/97 Studied chemistry at University of Göttingen, Degree Diploma

Scholarships and awards

- 2000 GlaxoWelcome scholarship
- 2008 Jochen-Block-Award 2008 of the DECHEMA
- 2012 DuPont Young Professor Award (2012-2014) (the only awarded European scientist)

Membership in advisory boards

- Since 2020 Speaker of the GRK2581 „Metabolism, topology and compartmentalization of membrane proximal lipid and signaling components in infection“
- Since 2020 Member of the Zentrum für Infektionsforschung, (ZINF), Würzburg
- Since 2019 Editorial Board member of the Journal *Scientific Reports*
- Since 2016 Editor in Chief, *Journal of Biosciences: Zeitschrift für Naturforschung C (ZNC)*, De Gruyter (Berlin, Germany)
- Since 2018 Board Member Professional School of Education, Würzburg
- Since 2018 Member of Common Graduation Commission of the Graduate School of Life Sciences
- 2011-2014 President of the German Society of Chemistry of lower Franconia
- 2011-2013 Member of the Faculty board of the Faculty of Chemistry and Pharmacy
- since 2012 Student counsellor for the Master programmes in Chemistry
- since 2013 Member of the study commission of Chemistry

Sphingolipids in infection

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Sphingolipids represent an important class of biomolecules that influence a wide range of biological functions. Implications of sphingolipids in diseases have garnered great attention in recent times and targeted intervention of sphingolipid turnover has proven to be a successful strategy in inflammation. However, its potential as a target in controlling infectious diseases at the level of metabolism and immune controls requires further definition. Incomplete elucidations of structure-to-function limit the ability to develop potent therapeutics. The lecture will present the development of novel approaches through a multi-disciplinary effort to study sphingolipids in infection

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Pradeep Singh obtained his BSc (1994), MSc (1996), and Ph.D. (2001) from the University of Madras. He was a post-doctoral fellow at the University of Cincinnati, USA, and at the University of Leeds, UK, before joining IITKGP in 2007.

His research interest is to design and develop one and two-photon responsive fluorescent PRPGs which can be operated in visible and NIR regions and to explore their applications towards photoresponsive DDSs for cancer treatment, NIR responsive donors for gasotransmitters, functional group photolithography, and controlled release of agrochemicals.

Prof. Singh is a recipient of the CRSI bronze medal (2020), SERB Distinguished Investigator Award (2018), a Member of the National Academy of Sciences (2018), and an Associate of the Indian academy of science (2009), etc.

1. Avijit Jana, K. Sanjana P. Devi, Tapas K. Maiti, and N. D. Pradeep Singh, Perylene-3-ylmethanol: Fluorescent Organic Nanoparticles as a Single-Component Photoresponsive Nanocarrier with Real-Time Monitoring of Anticancer Drug Release, *J. Am. Chem. Soc.*, **2012**, *134*, 7656-7659.
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Temporal Release of Cell Cycle Regulator α -lipoic acid: NIR-light Activatable Quinoxaline Based Nano-prodrug Delivery System

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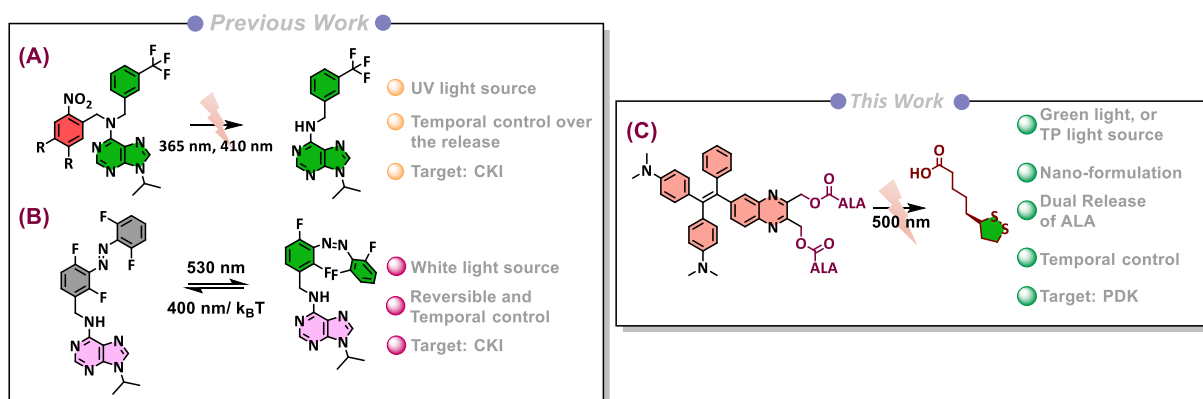
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The regulation of the cell cycle has recently opened up a new research perspective for cancer treatment. In this work, we have first synthesized a prodrug using a quinoxaline-based photoremovable protecting group (PRPG) to maintain the disrupted cell cycles by the temporal release of a well-known cell cycle regulator α -lipoic acid (ALA), using green light and NIR-light (Two-photon excitation). The suitable quinoxaline-based photocage of ALA has been formulated as fluorescent organic nanoparticles (FONs) and used effectively as a nano-DDS (drug delivery system) for better solubility and cellular internalization. Fascinatingly, the TP absorption cross-section of the nano-DDS was significantly increased (503 GM) compared to its bulk sample (384 GM), which signifies its utility for biological applications. Using green light, we have successfully controlled the time span of the cell cycles and cell growth of skin melanoma cell lines (B16F10) by the temporal release of ALA. Further, *in-silico* studies and PDH activity assay supported the observed regulatory behavior of our nano-DDS with respect to photo-irradiation. Overall, this approach expands the research path towards a futuristic photo-controlled toolbox for cell cycle regulation.

Figure/Scheme (if any):



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Education 1997 Habilitation in Experimental Physics, Heinrich-Heine-University Düsseldorf

1990 Dr. rer. nat., Heinrich-Heine-University Düsseldorf (Prof. D. Schmid):

Kohärenz und Relaxation von Singulett Excitonen in NaNO₂

1986 Diploma in Physics, Heinrich-Heine-University Düsseldorf

1979–1986 Study of Physics, Heinrich-Heine-University Düsseldorf

Academic Career since 2000 Professor of Physics (C4), University of Bayreuth

1999–2000 Professor of Physics (C3), LMU Munich

1990–1999 Postdoctoral Fellow at the “Centre for the Study of Excited States of Molecules”, Leiden University (Netherlands)

1997–1999 Heisenberg Fellow (Prof. J. Schmidt), Institute of Physics, Leiden University (Netherlands)

1990–1996 Postdoc (Prof. J. Schmidt), Institute of Physics, Leiden University (Netherlands)

1987–1990 Research Associate (Solid State Physics), Faculty of Mathematics and Natural Sciences, Heinrich-Heine-University Düsseldorf

Research Topics

Optical spectroscopy of soft condensed matter; Single-molecule spectroscopy; Energy and charge transfer processes in molecular aggregates and (artificial) photosynthetic light-harvesting systems

Honors & 2019 Wilsmore Fellowship, University of Melbourne

Awards 2002 Chair offered from University of Linz (Austria, declined)

1997 “Richard Heynen – und Emmy Heynen Prize” by the Society of Friends and Promoters of the Heinrich-Heine-University Düsseldorf

1997 Grant “Heisenbergstipendium” (DFG)

1996 Gustav-Hertz-Prize of the German Physical Society (DPG)

1995 Grant “Habilitationstipendium” (DFG)

1994 C.J. Kok Prize, Leiden University (Netherlands)

1991 Best Dissertation of the Year, Heinrich-Heine-University Düsseldorf

The light harvesting complex of the marine alga *Codium fragile*. Spectroscopy of single siphonaxanthin-siphonein-Chl-a/b-proteins (SCP): A Status Report

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The siphonaxanthin-siphonein-Chl-a/b-protein (SCP) complex is the major light-harvesting antenna from the siphonous green alga *Codium fragile* and is highly homologous to the light harvesting complex LHCII of higher plants. Yet, *Codium fragile* is a macro algae that lives in intertidal zones that feature unique irradiation conditions. While for land plants (LHCII) excess light comes at irregular timings and features a white spectrum, under water sudden intensity changes are diminished, and excess light features a red-enhanced spectrum that comes at tidal timings. We have recorded simultaneously the spectral peak position of the emission and the fluorescence lifetime from single SCP complexes for two different excitation wavelengths, namely 561 nm (green) and 639 nm (red). For excitation in the green spectral range we find for most of the complexes "normal" LHC II - like spectral features, i.e. an emission peaking around 680 nm and fluorescence lifetimes between 3 ns and 4 ns. In contrast, excitation in the red spectral range yields a red-shifted emission peaking between 690 nm - 720 nm and lifetimes around 2 ns. We suggest that the difference in response of SCP to light of 561 nm and 639 nm reflects the adaption of the algae to the natural habitat, and hypothesize that this is associated with a transition to the photoprotection mode.

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R. Madhan

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Mr. R. Madhan has taken over the position to lead the bilateral Indo-German Science and Technology Centre (IGSTC) as its Director on 29th December 2020 and has been actively catalyzing Indo-German Science & Technology partnerships. Mr. Madhan during his tenure as Director, IGSTC had expanded the programme portfolio of IGSTC for providing opportunities to a large community including early career, mid-career and cross gender representation. He had initiated major programmes to enhance involvement of Indo-German Scientific communities and to foster strategic partnerships.

The new programmes initiated were IGSTC Industrial Fellowship (IF) for industrial exposure in Germany for young Indian researchers, Women Involvement in Science and Engineering Research (WISER) to facilitate lateral entry for women in STEM, Paired Early Career Fellowship in Applied Research (PECFAR) for creating avenues for two-way exchange of young research in pairs and Small Immediate Need Grants (SING) for providing quick assistance to kick off ad-hoc opportunities with fast track processing. He also added an important aspect as per the IGSTC's mandate to strengthen public-private partnerships by developing academia-industry connect programmes to foster industrial research, innovation and entrepreneurship and forged tie-ups with industries like BASF and TATA Steel.

He had earlier been associated with development of marine instrumentation and autonomous underwater technology for oceanographic research at CSIR-National Institute of Oceanography (NIO), Goa from 1991 to 2020. As a Chief Scientist and Head of the Marine Instrumentation Department at CSIR-NIO, he has contributed in the development of several marine robots including Autonomous Underwater Vehicle (AUV)-MAYA, remotely operated surface vehicles and autonomous vertical profilers (AVP). He played a key role in transferring AUV and AVP technology know-how to industry and in commercialization of the same. He had also played a major role in capacity building and popularizing marine robotics in India.

Mr. Madhan had also served as the Science Counselor at the Embassy of India, Berlin, Germany for three years during which he ably facilitated, coordinated and contributed in enhancing bilateral cooperation between India and Germany. He played a major role in connecting scientists and academicians of India & Germany on several areas including clean energy, next generation batteries, high energy physics, marine robotics, biotechnology, molecular biology, space research, climate research, education and sustainable studies. He contributed significantly in connecting German institutions (including Fraunhofer, Leibniz, Helmholtz, Max Planck Institutes, TU9, Excellence Initiative Universities) with Indian counterparts (including CSIR, DBT, DST, MoES, ICAR, IISc, IIT).

His experience with international partners includes work with the Institute for System and Robotics (ISR), Instituto Superior Técnico (IST), Lisbon through the Indo-Portuguese bilateral project on marine technologies and the Monterey Bay Aquarium Research Institute, California through the POGO-SCOR fellowship. He is the recipient of the Meritorious Invention Award from the National Research Development Corporation (NRDC), Ministry of S & T, New Delhi for "Autonomous Vertical Profiler (AVP)" for the year 2010. He is a Fellow of the Institution of Engineers, India. His research career following the Electrical & Electronics Engineering degree from REC, Calicut and Master's degree in Power & Energy systems from REC, Surathkal has resulted in several publications in journals and conferences in addition to international patents.

Indo-German Science & Technology Centre (IGSTC)

R. Madhan

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The Indo-German Science & Technology Centre (IGSTC), a joint initiative by the Department of Science & Technology (DST), Government of India and the Federal Ministry of Education and Research (BMBF), Government of Germany was established to facilitate Indo-German R&D networking through substantive interactions among government, academia/research system and industries, thus fostering innovation for overall economic and societal developments in both the countries.

IGSTC is actively involved in

1. Facilitating and promoting Indo-German bilateral collaborations in basic and applied science, research and technology
2. Encouraging public-private partnerships (PPP) to foster elements of innovation and industrial application and cultivating a culture of cooperation between science and industry.
3. Nurturing contacts between young and mid-career scientists and technologists to develop a sense of mutual trust, partnership/leadership and entrepreneurship.

Currently IGSTC is offering various opportunities for R&D&I, networking, and long-term collaboration between academia & industries.

1. **2+2 Programme:** IGSTC intends to catalyse innovation centric R&D&I projects by synergising the strength of research/academic institutions and industry from India and Germany. 2+2 programme is aimed at supporting joint R&D&I projects of industrial relevance by means of “2+2 Mode of partnership” i.e involvement of at least one research/academic institution and one public/private industry from both the countries.
2. **IGSTC Open Call Workshop:** The Bilateral Workshops aim towards creating a platform for substantive interaction between scientists/researchers from academia and industry in state-of-the-art S&T areas.
3. **IGSTC Industrial Fellowships:** This Fellowship programme is tailored for PhD students and post-doctoral researchers in S&T with appreciable track record and aptitude for applied research & technology development. It is designed to provide a short-term exposure to researchers at an early stage of their career in a German industrial setup.
4. **Women Involvement in Science & Engineering Research (WISER):** The programme is a first of its kind programme that intends to build scientific capacity, retain and promote women researchers in India/Germany by utilizing complementary expertise in science, technology, innovation and research partnerships.
5. **Paired Early Career Fellowship in Applied Research (PECFAR):** This fellowship facilitates a two-way exchange of early career Indian and German researchers in a ‘pair’ to have a short duration visit to explore, connect and network for research collaborations in frontier areas of Science, Technology, Engineering and Mathematics (STEM).
6. **Small Immediate Need Grants (SING):** The programme aims to provide quick & immediate grant to proposals/initiatives that requires modest funding to embark on Indo-German bilateral scientific & research collaboration.
7. **IGSTC CONNECT-Plus:** Alexander von Humboldt Foundation (AvH) supports participants of the Indo-German Frontiers of Engineering Symposia (INDOGFOE) through a follow-up programme CONNECT that facilitates research stays of INDOGFOE participants. IGSTC CONNECT-Plus is a mobility grant for successful Indian and German CONNECT awardees to promote scientific exchange and networking.

Reference: www.igstc.org

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Education and Employment History

<u>Institution</u>	<u>Degree</u>	<u>Period</u>
University of Iceland	B.S. (Chemistry)	9/82-5/87
University of Washington	Ph.D. (Organic Chemistry)	9/88-12/93
Max-Planck-Institut für experimentelle Medizin, Germany	Postdoctoral Research Associate	1/94-6/96
University of Washington	Research Assistant Professor	9/96-6/03
University of Washington	Research Associate Professor	7/03-9/04
University of Iceland	Professor	3/02-pres.

Recent representative publications

Gränz M, Erlenbach N, Spindler P, Gophane DB, Stelzl LS, Sigurdsson ST, Prisner TF, "Dynamics of nucleic acids at room temperature revealed by pulsed EPR," *Angew. Chem. Int. Ed.* **57**, 10540-43 (2018).

Mentink-Vigier F, Marin-Montesinos I, Jagtap AP, Halbritter T, van Tol J, Hediger S, Lee D, Sigurdsson ST, De Paëpe G, "Computationally-assisted design of polarizing agents for dynamic nuclear polarization enhanced NMR: the AsymPol family," *J. Am. Chem. Soc.* **140**, 11013-9 (2018).

Collauto A, von Bülow S, Gophane DB, Saha S, Stelzl L, Hummer G, Sigurdsson ST, Prisner TF, "Compaction of RNA duplexes in the cell," *Angew. Chem. Int. Ed.* **59**, 23025-23029, (2020).

Harrabi R, Halbritter T, Aussenac F, Dakhlaoui O, van Tol J, Damodaran K, Lee D, Paul S, Hediger S, Mentink-Vigier F, Sigurdsson ST, De Paëpe G, "Highly efficient polarizing agents for MAS-DNP of proton-dense molecular solids," *Angew. Chem. Int. Ed.*, **61**, e202114103 (2022).

Improving the sensitivity of NMR spectroscopy with stable radicals

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Structural determination of biomolecules at the atomic level can provide functional insights that are necessary for rational design of modulators and inhibitors of biological function. Nuclear Magnetic Resonance (NMR) spectroscopy is a prominent technique for this purpose, but the low sensitivity of NMR limits its use for the study of biomolecules, in particular within living cells. In recent years, this drawback has been addressed by using Dynamic Nuclear Polarization (DNP),¹ a hyperpolarization technique that utilizes microwave-assisted transfer of spin polarization from radicals (polarizing agents) to the nuclei of interest. The sensitivity gain conferred by DNP enables the study of biomolecules and drugs at their physiological concentration.² Nitroxide biradicals such as AmuPol,³ bcTol-M,⁴ and AsymPol-POK⁵ (**Figure 1**) are examples of effective polarizing agents for high-field DNP NMR. The design, synthesis and properties of polarizing agents that have been developed in our laboratory will be described, along some challenges that still remain.

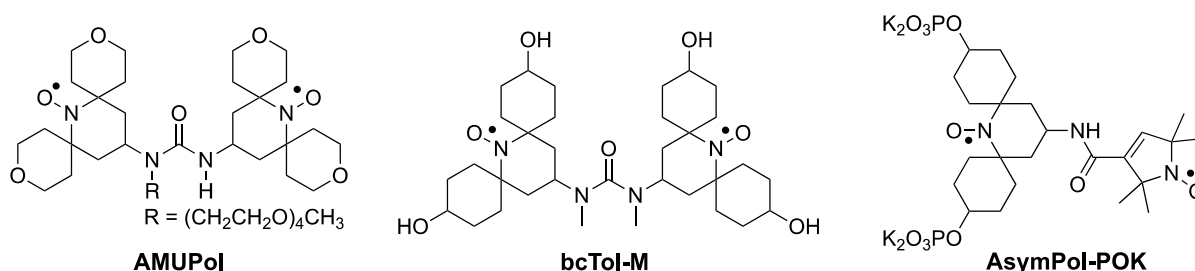


Figure 1. Binitroxide polarizing agents for DNP NMR.

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3. Sauvee, C.; Rosay, M.; Casano, G.; Aussenac, F.; Weber, R. T.; Ouari, O.; and Tordo, P. *Angew. Chem. Int. Ed.* **2013**, *52*, 10858-10861.
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Dr. Gardas' research group focuses on 'Chemical Thermodynamics' and 'Phase Equilibria' of industrially important solvents and their mixtures. His research group focuses on both 'Science' and 'Technology' part of the contemporary field – "Ionic Liquids/ Deep Eutectic Solvents as an alternative to Volatile Organic Solvents" and significantly contributes to connecting them. His research group substantially contributed to the development of non-conventional and environmentally benign solvent systems. Generated extensive databases on their thermodynamic properties and structure-composition-property correlations useful in refrigeration, separation science, and crude oil industry. These will have far-reaching implications in the design of application-specific solvent systems, such as phase change materials, CO₂ capturing, dissolution of tank bottom sludge, electrolytes in solar cell and supercapacitors, absorbents for refrigeration system, desulfurization of fuels, and also the extraction of metal ions, biomolecules, and value-added products. More than 17,500 thermodynamic data points measured in his research lab at IIT Madras are included in NIST Standard Reference Database developed by Thermodynamics Research Center, NIST, USA.

Dr. Gardas has more than 21-years of research and 12-years of teaching experience. So far, he has completed 8 projects (as PI and Co-PI) worth more than Rs. 6.5 crores, guided 14 Ph.D. and 17 M.Sc. project students. Co-authored 4 patents, 11 book-chapters, 7 conference papers, 4 Editorials, and 195 research publications which received more than 7575 citations with h-index = 44. He has delivered more than 250 invited talks and guest lectures.

In recognition of his outstanding performance as a researcher, Dr. Gardas has been bestowed with several awards by prestigious institutes/ societies, including the Mid-Career R&D Award-2020 by IIT Madras. Recently, he has been recognized as (i) Associate Editor of an American Chemical Society Journal, Journal of Chemical & Engineering Data, (ii) Fellow Royal Society of Chemistry (FRSC), UK, (iii) Asian Thermophysical Properties Research (ATPC) Significant Contribution Award 2022, (iv) Publons Top Peer Review Award 2019 (Top 1% of Reviewers in Chemistry), and (v) Featured in the list of "World Ranking of Top 2% Scientists" in 2021 database created by experts at Stanford University, USA.

Benign Solvents as Performance Additives to Enhance the Extraction of Micropollutants and Heavy metals

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Despite many waste management strategies, the amount of chemical pollutants in the environment is constantly rising. Concerning water treatment, the removal of micropollutants from water bodies remains elusive. Micropollutants (MPs) are chemicals that occur in trace amounts in the aquatic environment, which include pharmaceuticals, food additives, cosmetics, and dyes¹. The presence of MPs in the aquatic environment has been associated with many adverse effects, including biomagnification, undesirable mutation, and genotoxicity. The need to develop sustainable and cost-effective alternatives to eliminate these toxins has become a pressing issue. Apart from this, the rapid technological changes and the short life span of electronic devices create an abrupt accumulation of electrical and electronic waste (WEEE) in the environment. The heterogeneity of constituents in e-waste and the presence of hazardous materials raise complexity in e-waste treatment². Recently, ionic liquids (ILs) have emerged as a promising possibility for task-specific, efficient pollutant extraction because of the ease in structure tunability and other unique chemical properties³. Deep eutectic solvents (DES), often referred to as a subclass of ILs, were also widely renowned for pollutant extraction capability⁴. Our research studies recently found that alkanolamine-based ILs are potential performance additives to eliminate pharmaceutical micropollutants in the aquatic environment, and choline chloride-carboxylic acid DES are an alternative to the conventional leaching acids for the recovery of valuable metals from e-waste. DFT studies based on Gaussian 16 support the experimental data and further illustrate the potential of these alternative solvents. The proposed methodologies for extraction are rapid and facile without compromising environmental concerns.

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Josef Wachtveitl studied Physics at Regensburg University and obtained his PhD in Bioenergetics from the Max Planck Institute of Biochemistry in Martinsried in 1992. He then moved to Ludwig Maximilian University of Munich, where he worked as a postdoc at the Institute of Medical Optics. During this postdoc he also spent time at the Argonne National Laboratory, USA and the Centre d'Études Nucleaires de Saclay, France. He habilitated in physics in 1998 and was appointed Professor (C3) for Physical Chemistry at Goethe University in 2000. In 2004 he was promoted to C4. From 2004 to 2010 he was also a professor at the Institute of Biophysics and co-founded the biophysics course at Goethe University which started in 2008.

Currently he is member of the DFG review board (FK 323, Physical Chemistry) and vice-dean and dean of research of the Faculty Biochemistry, Chemistry and Pharmacy.

His research interests include time resolved optical and vibrational spectroscopy, femtochemistry, structure and function of photoreceptors, molecular mechanisms of photoresponses in retinal protein, conformational dynamics of biopolymers, protein folding, RNA dynamics, photosynthetic energy conversion, interfacial electron transfer and light responsive model systems.

Publications (<https://orcid.org/0000-0002-8496-8240>)

1. Trinh, P. T., Hasenstab, S., Braun, M. and Wachtveitl, J. (2022) *Ultrafast separation of multiexcitons within core/shell quantum dot hybrid systems*, **Nanoscale**, **14**, 3561-3567
2. Asido, M., Hamerla, C., Weber, R., Horz, M., Niraghatam, M.S., Heckel, A., Burghardt, I. and Wachtveitl, J. (2022) *Ultrafast and Efficient Energy Transfer in a One and Two-Photon Sensitized Rhodamine-BODIPY Dyad: A Perspective for Broadly Absorbing Photocages*, **Phys. Chem. Chem. Phys.**, **24**, 1795-1802
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Azobenzene photoswitch scaffolds: scope and (bio-)molecular applications

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Molecular photoswitches are versatile tools that offer a highly selective, spatiotemporally precise and non-invasive way for control of nanosystems. Azobenzenes (ABs) are a major class of photoswitches with photochromism based on the E \leftrightarrow Z isomerization of their N=N bond. Suitably connected to biomolecules, azobenzenes can act as light trigger for initiation of conformational transitions. Introduction of photoswitches into peptides, nucleic acid constructs and proteins allows photocontrol of the operation of such biomacromolecules and reprogramming of their response.[1] Recently, we studied the dynamics of ligand-protein interactions by ultrafast spectroscopy and time-resolved serial crystallography.[2] The release of the photopharmacological compound azo-combretastatin from $\alpha\beta$ -tubulin, the principal building block of the microtubule cytoskeleton could be observed. Microtubules have pivotal roles in cell division and survival and $\alpha\beta$ -tubulin targeting agents are potent drugs widely used in chemotherapy and cancers treatment.

ABs have also been implemented in complex photoresponsive nanostructures and materials. Furthermore, studies on the ultrafast isomerization dynamics of substituted[3,4] and multichromophoric[5] systems (bis- and tris-azobenzenes) provide a deeper understanding of the photophysics and photochemistry of the individual building blocks and open the way to an intelligent design of complex photoswitchable nanostructures.

On a different note, AB is also a promising candidate for conversion of solar energy, since it can be converted from a low energy structure to a meta-stable higher energy isomer upon absorption of solar irradiation and the stored energy can then be released on demand by an external trigger. Especially multi-ABs allow the design of efficient photoconverting molecules with high energy storage density with a long half-life of the high energy state.

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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.
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Development of N-Heterocyclic Carbene Complexes of Cobalt for Carbon-Boron Bond Formation

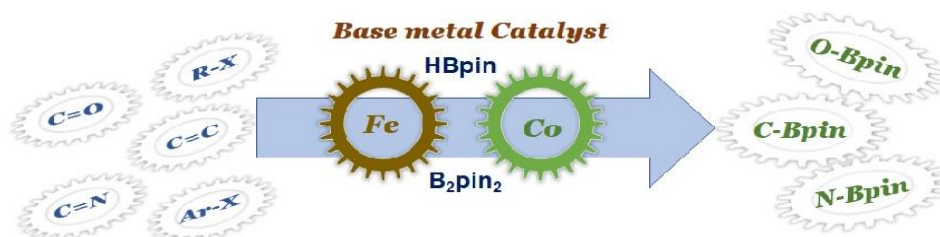
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Given their importance in utility as versatile precursors to a wide range of other valuable families of molecules, introducing diverse functionality into the organoboron compounds will enhance its use as a synthetic handle in target-directed synthesis.¹ 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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Tomáš Slanina did his PhD in 2015 as a joint degree between the groups of Prof. Petr Klán at MU Brno, Czech Republic and Prof. Burkhard König and UR Regensburg, Germany. After two postdoctoral stays with Prof. Alexander Heckel at Goethe University, Frankfurt am Main, Germany, and with Prof. Henrik Ottosson at Uppsala University, Sweden, he started his independent research group in 2019 at the Institute of Organic Chemistry and Biochemistry in Prague, Czech Republic. The group focuses on redox photochemistry, a novel research field that combines the photochemistry of small molecules with redox processes relevant to photocatalysis.

Tomáš Slanina is a co-author of 32 publications in leading journals (e.g., *J. Am. Chem. Soc.*, *Angew. Chem. Int. Ed.*, *Chem. Sci.*) that have been cited >1400 times (h-index: 17). He received several awards, among others Alfred Bader Organic Chemistry Prize (2019), European Photochemistry Association Prize (2016), Jean-Marie Lehn PhD. Chemistry Prize (2015). He was awarded the ERC Starting Grant in 2021 for a project developing organic solar batteries.

Reversibility in Photochemistry: Beyond the Classical Approaches

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Compounds that can be interconverted between two forms, **A** and **B**, reach a chemical equilibrium dictated by the relative stabilities of the respective forms. Chemists have always been fascinated by the possibility of fighting this equilibrium using external triggers to quantitatively convert **A** to **B** and vice versa. Our approach uses light of different wavelengths to switch a molecule between two states (Fig. 1).

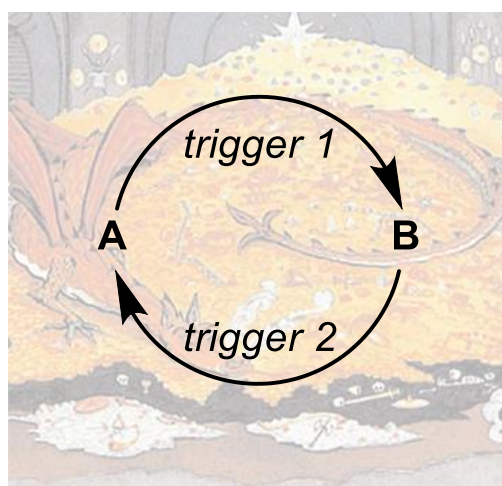


Figure: Reversible switching between two molecules by external triggers.

We optimise the photochemical switching properties of existing diarylethene¹ and fulgimide² systems and develop water-soluble photoswitches that can be applied in photopharmacology to alter the properties of biologically active substances reversibly. In addition, we develop entirely new reversible systems based on photoinduced electron transfer (“electron ping-pong”) and reversible formation and cleavage of a σ -bond through ortho-quinone methides (“catch-and-release”). These approaches broaden the scope of reversible photochemical systems applied in optogenetics and material chemistry.

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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 Indian Association for the Cultivation of Science (Thesis 2010) and postdoctoral training at the Emory University. From Jan 2017, he is working in IISER Kolkata. Dibyendu leads an interdisciplinary group that focuses on designing active and adaptive materials by harnessing non-equilibrium self-assembly and exploring the functional materials under the purview of systems chemistry. His lab is invested in mimicking how living systems work from the perspective of the emerging and young field of systems chemistry. The intelligence and autonomy of living matter keep inspiring his research to attempt synthesizing materials with adaptive properties.

Awards and Distinctions

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

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Living Matter Like Materials via Complex Chemical Systems

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There remain critical gaps in our understanding of the emergence of functional biopolymers in the origins of Earth's biosphere. Extant proteins, evolved over millions of years, carry out an impressive array of responsibilities, from catalysis and molecular recognition to motility and compartmentalization. One of the major goals of our lab is to investigate the possible origins of advanced enzymatic functions from folds of short peptide based paracrystalline phases. 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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10. S. Bal, K. Das, S. Ahmed and D.Das* *Angew. Chem. Int. Ed.* **2019** 58 244.
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Surajit Ghosh was born in West Bengal, India. He studied Organic Chemistry at the University of Calcutta, India, and gained his Master of Science in Organic Chemistry in 2000. Then, he moved to Syngene International Pvt. Ltd (Biocon INDIA Group) and worked as a Scientist till July 2004 in drug discovery project. Subsequently, he moved to Indian Institute of Technology, Kanpur in August 2004 for his doctoral studies in the group of Prof. Sandeep Verma in the area of Peptide Self-assembly. After completing his Ph. D. in July 2008, he received postdoctoral fellowship at Cell Biology and Biophysics Division of European Molecular Biology Laboratory, Heidelberg, Germany with Dr. Thomas Surrey (August 2008), where he worked on organization of microtubule and molecular motor proteins till December 2010. He joined CSIR-Indian Institute of Chemical Biology Kolkata, India in 2011, and worked as Principal Scientist till July 2019. Subsequently, he has joined as Professor in the Department of Bioscience and Bioengineering at Indian Institute of Technology Jodhpur on July 2019. He is a recipient of BIOCON Tribute award, EMBL Fellowship, Alexander von Humboldt Fellowship, Ramanujan Fellowship, Indian Peptide Society Young Scientist Award, Asima Chatterjee Young Scientist Award, CSIR-CDRI Award for Excellence in Drug Research (2020) and SERB-STAR Award (2020). He is an elected Fellow of Royal Society of Chemistry (2016), and West Bengal Academy of Science and Technology (2018). He served as Dean (Research and Development) at IIT Jodhpur (Sep 2019-Aug 2022). Recently, he became editorial board member of RSC Advances (2022) and serving as Associate Editor of RSC Advances (2015-2025) and Frontiers of Chemistry (Chemical Biology). At IIT Jodhpur he is leading his group with a current research focus on the areas of Chemical Neuroscience, Chemical Biology and Development of Biophysical Platform/Biosensor.

Engineered Antimitotic Peptide Evolved from Hotspots of Tubulin Interface

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Protein-protein interactions play a crucial role in microtubule dynamics. Microtubules, key cytoskeleton filaments are considered as a key target for the design and development of anticancer therapeutics, where inhibition of tubulin-tubulin interactions plays a crucial role. Here, we focused on a few key helical stretches at the interface of α,β -tubulin heterodimers and developed a structural mimic of these helical peptides, which can serve as potent inhibitors of microtubule polymerization. To induce the helicity in these sequences, we have made stapled analogues of these sequences. Thereafter, we modified the lead sequences of the antimitotic stapled peptides with halo derivatives. It is observed that halo-substituted stapled peptide follows an interesting trend of the order of halogen atoms electronegativity in interaction patterns with tubulin and a correlation in toxicity profile. Remarkably, we found that para-fluoro phenyl alanine modified stapled peptide is the most potent inhibitor, perturbs microtubule dynamics, induces apoptotic death, and inhibits the growth of the tumor.¹

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CAREER

04.2006 – 03.2015 Founder and Coordinator of the GRK 1221: Control of Electronic
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07.2003 – 06.2015 SFB 630: Recognition, Preparation and Functional Analysis of Agents
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04.2001 – 03.2004 Founder and Coordinator of GRK 690, Electron Density: Theory and
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04.1999 – current Professor of Theoretical Chemistry (W2)
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03.1992 – 03.1999 Scientific Assistant (C1), University of Bonn
01.1990 – 02.1992 Postdoctoral Researcher with Prof. S.D. Peyerimhoff, University of Bonn
01.1989 – 12.1989 Postdoctoral Researcher with Prof. F. Grein, University of New
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EDUCATION

09.1987 – 02.1992 Habilitation in Theoretical Chemistry, Rheinische Friedrich-Wilhelms-
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Hyperfine coupling constants of molecules*
09.1985 – 08.1987 Dr. rer.nat. awarded by the University of Bonn; Doctoral research work
on
ESR constants of small molecules in the group of Prof. S.D. Peyerimhoff
09.1978 – 08.1985 Study of Chemistry and Theoretical Chemistry at the Universität Bonn

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Boron Chemistry

What Can Theory Contribute New and What to Pay Attention to For Accurate Calculations

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Boron chemistry has made tremendous progress in recent decades, leading to the isolation of a variety of compounds with remarkable electronic structures and properties. To stabilize such compounds, Lewis bases are of tremendous importance. Cyclic (alkyl)(amino) carbenes (CAACs) and N-heterocyclic carbenes (NHCs) are widely used, leading to compounds with closed shells but also with biradicaloid electronic structures. In this talk, we explore the underlying effects that determine the electronic structures of each species and show how UV-Vis spectra can be used to accurately characterize the electronic structure of biradicaloid electronic structures.¹⁻⁴

In addition, we focus on anionic boron and carbon-based hetero-biradicaloids to uncover the reasons for their small singlet-triplet gaps.^{5,6} For the various examples, we always highlight potential pitfalls in the calculations.

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Ravi P. Singh born in Ghazipur, UP, is currently professor in chemistry department at the Indian Institute of Technology (IIT) Delhi, India. He obtained his Bachelor's degree in chemistry from U.P. College, Varanasi and Master's degree from Banaras Hindu University, Varanasi. Later, he moved to the Chemistry Department at IIT Kanpur, to pursue his Doctoral studies under the supervision of Prof. Vinod K. Singh. He gained his postdoctoral experience in U.S.A in the area of total synthesis and asymmetric catalysis. Dr. Singh spent two years (2005-2007) at Harvard University working with Nobel Laureate, Professor E. J. Corey and four years (2007-2011) at Brandeis University working with Professor Li Deng. He started his independent academic career at National Chemical Laboratory - Pune as a Senior Scientist in 2011 and later moved to the chemistry department at IIT-Delhi in 2013. Prof. Singh's research interest is broadly in the field of synthetic organic chemistry and specifically in Asymmetric Catalysis, C-H Activation and total synthesis of small molecules. His research group is not only pursuing various ways to make and break C-C and C-X bonds but also trying to develop strategies to synthesize biologically active and other pharmaceutically relevant natural products in a cost effective way.

Dehydrogenative C-C and C-P Bond Formation

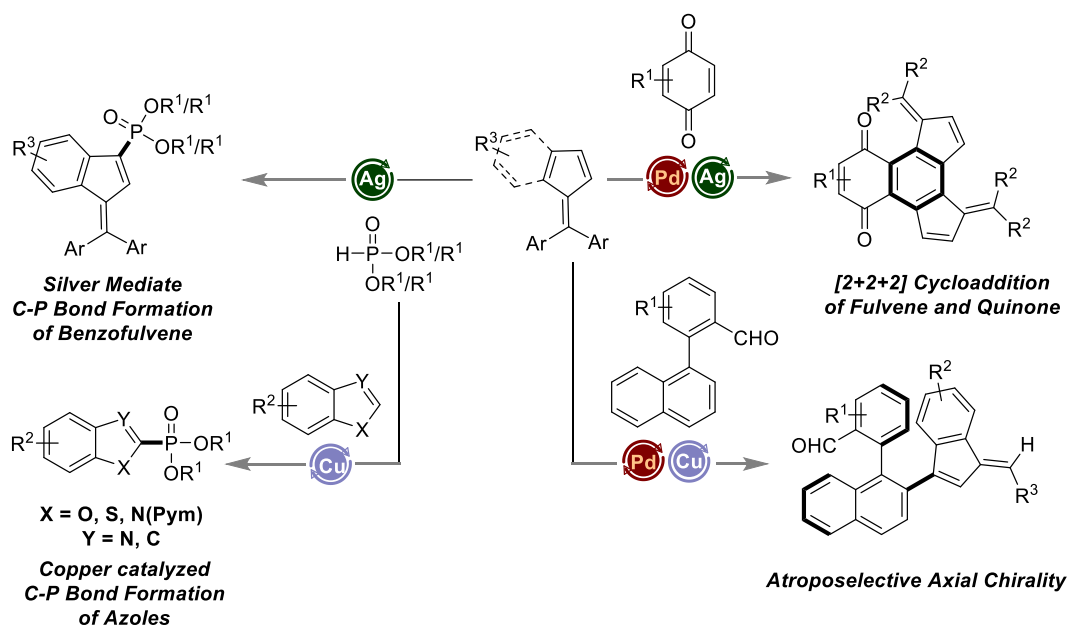
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Selective organic transformation, be it chemo-, regio- or stereoselective carbon-carbon and carbon-heteroatom bond formation is most challenging to achieve. Thus, developing strategies for generating C-C bond and C-phosphorous is critical in the design and synthesis of organic matter. In this context, a potent new method for synthesising compounds, transition metal catalysed cross-dehydrogenative coupling (CDC) or oxidative coupling has recently evolved as a powerful tool in organic synthesis.¹ Here, a ligand free Cu-catalysed C-P bond formation by hetero cross dehydrogenative coupling reaction between P(O)-H and hetero C-H bonds along with Ag-mediated direct C-3 phosphorylation of electron rich benzofulvene moieties has been explored.² Moreover, another regio-selective C-H activation of fulvene in terms of [2+2+2] cycloaddition between quinones and fulvenes using oxidative ligand-assisted palladium catalysis to synthesize numerous polyarylquinones has been developed.³ It was found that, synthesized polyarylquinones exhibits the potential to serve as an either antioxidant or chemotherapeutic agent. Finally, utilizing imines as the transient directing group for bi-aryl aldehydes to gain axially chiral bi-aryls containing benzofulvenes using palladium catalysis is also demonstrated.



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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.
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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.
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9. C. Yang, C. Slavov, H. A. Wegner, J. Wachtveitl, **A. Dreuw**, *Chem. Sci.* **2018**, *9*, 8665
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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.

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RESEARCH EXPERIENCE

2019-present: Assistant Professor, Materials Research Centre, Indian Institute of Science, Bangalore, India

2016-2019: Marie Curie Fellow (Advisor: Prof. Eli Zysman-Colman and Prof. Ifor D. W. Samuel), Organic Semiconductor Centre, University of St Andrews, UK.

2012-2016: Post-doctoral fellow (Advisor: Prof. Chien-Hong Cheng), National Tsing Hua University, Taiwan.

2008-2012: Ph.D. in Chemistry (Advisor: Prof. Edamana Prasad), Indian Institute of Technology Madras (IITM), India.

AWARDS/RECOGNITION

2022: IGSTC-WISER award

2021: Rekha Rao Young Investigator award

2017: Marie Sklodowska-Curie individual Fellowships

2016: DST Inspire Faculty Award.

2012: National Science Council Postdoctoral Fellowship (NSC), Taiwan.

2013: Prof. Ramamurthy award for the best Ph.D. thesis in Chemistry, IIT Madras.

PROFESSIONAL OUTCOMES

Total no of publication: 40 (journal papers) and 4 patents

Total no of Citation: 2084

h index: 23

i10 index: 29

Organic Thermally Activated Delayed Fluorescence Emitters for Organic Light Emitting Diodes

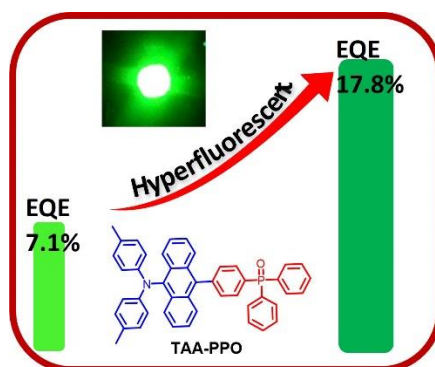
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Many applications such as bioimaging, displays and lighting benefit from the development of luminescent materials. In recent years, thermally activated delayed fluorescence (TADF) have emerged as promising emitters for organic light emitting diodes (OLEDs) for displays and solid-state lighting.¹ The most exciting feature of TADF-OLEDs is the harvesting of triplet excitons using a purely organic dye molecule with efficient reverse intersystem crossing (rISC). Here, we systematically designed and synthesized TADF emitters with various benzoyl pyridine ketones to develop efficient OLEDs. An electroluminescent device of one such dopant shows an external quantum efficiency (EQE) of 25% with deep blue emission.² New TADF molecular design strategy for high performance ultrathin non-doped OLEDs and improved device performance of conventional fluorescence emitter using TADF as an assistant dopant.^{3,4}



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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>

Young *et al.* Sci Rep 10, 20398 (2020).
<https://doi.org/10.1038/s41598-020-76867-9>

Lieblein *et al.* eLife 2020;9:e59306
<https://doi.org/10.7554/eLife.59306>

Hellwig *et al.* Chemical Communications 54, 13702-13705 (2018),
<https://doi.org/10.1039/C8CC06284F>

Henrich *et al.* eLife 6, (2017).
<http://dx.doi.org/10.7554/eLife.20954>

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- β 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 complex¹, or the weak point in the Amyloid- β assembly², which allows to disrupt this process.

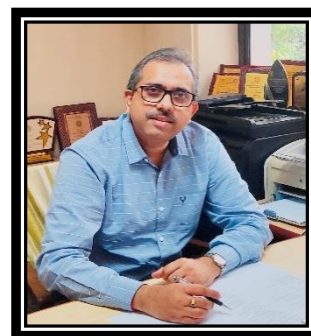
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Career Profile:

2015- present *Senior Professor, IACS*
2010-2015 *Professor, IACS.*
2006-2010 *Associate Professor, IACS*
2005-2006 *Assistant Professor, IACS*
2002-2005 *Senior Lecturer, IACS*
2000-2002 *Post-Doctoral Research, Massachusetts Institute of Technology (MIT), USA*
1995-1999 *PhD, CSIR-Indian Institute of Chemical Technology/Osmania University, Hyderabad*

Awards/Achievements and Fellowships:

- Featured in '75 under 50' Scientists Shaping Today's India – 2021
- Fellow, Indian Academy of Sciences (FASc) - 2017
- Materials Research Society of India (MRSI) Medal - 2017
- Highlighted Author by ACS for Publishing High Quality Research in ACS Journals – 2012
- CRSI (Chemical Research Society of India) Bronze Medal – 2011
- Ramanna Fellowship Award of DST, India – 2006-2009
- B. M. Birla Science Prize in Chemistry – 2006
- Fellow, West Bengal Academy of Science & Technology (FAScT) – 2008

Publications:

1. *Langmuir* 2022, 38, 3480-3492.
2. *Langmuir* 2019, 35, 15180-15191.
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Organic Nanostructures in Cellular Transportation

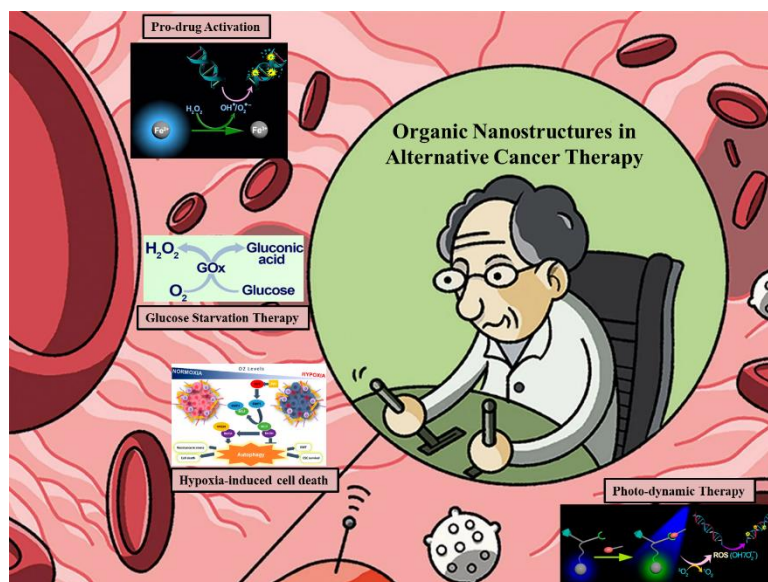
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With the rapid development of nanotechnology, the convergence of nanostructures and drug delivery system (DDS) has become a research hotspot in recent years. Due to their unique and superior properties, various organic nanostructures are able to significantly increase the solubility of drugs, reduce cytotoxicity, and improve therapeutic efficacy. They have been used *in vivo* to protect the drug entity in the systemic circulation, control access of the drug to specific targeted sites in a sustainable manner. In cancer therapy, one of the main component of these DDS is the presence of an anti-cancer drugs within it. These systems have limitations that leads to explore alternative therapy. The primary emphasis of alternative cancer therapy is the utilization of target-specific theranostic agents that can itself diagnose as well as treat cancer cells selectively without the assistance of anti-cancer drugs. In this perspective, our lab's approach includes various alternative cancer research such as glucose starvation therapy, pro-drug activation, photo-dynamic therapy and hypoxia-induced killing of cancer cells.¹⁻⁶ The significance of constructing organic nanostructures with their enhancing role in DDS by exploring unconventional therapy will be presented in this lecture.



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Dr. Nidhi Gour obtained her Ph.D. in Organic Chemistry from IIT Kanpur in 2010 under the kind supervision of Prof. Sandeep Verma. Her Ph.D. thesis was awarded with the second prize of Eli Lilly Asia Outstanding Thesis Award. After two short post-doctoral stints at Tata Institute of Fundamental Research (TIFR), Mumbai and Albert Einstein College of Medicine, New York, USA, she joined the University of Geneva, Switzerland as post-doctoral fellow for two years and finally CSGI, University of Florence for one year. Thereafter she joined as an Assistant Professor in Indian Institute of Advanced Research as full time Faculty in August 2016. In July 2019 she joined Indrashil University (IU) where she is currently working as Associate Professor. Dr. Nidhi's research is based on studying molecular self-assemblies and assessing its implications in biology and material science. Her research as Faculty and main corresponding author has been published in reputed Q1 journals like Current opinion in Chemical Biology, ACS Chemical Neuroscience, ACS Applied Biomaterials, New Journal of Chemistry and Soft Matter. The research publication of her group has been cited in high impact Journals like Nature Nanotechnology and ACS Nano. She is also serving as a reviewer for ACS, RSC, Elsevier and Springer Journals and serves as a reviewer for Israel Science Foundation (ISF) Grant. She has also served as Coordinator for national and international workshops and conferences like DST INSPIRE Science camp, IU webinars, GujCOST webinars and International e-conference.

Metabolite amyloids and its possible implications in disease etiology

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The word “amyloid” was conventionally referred to as abnormal aggregates of proteins and peptides which produced cellular toxicities and caused pathogenesis in protein misfolding diseases like Alzheimer’s and Parkinson’s to name a few. However, recent research suggest not only proteins and peptides but metabolites like single amino acids,^{1a} nucleobases,^{1b} glucosylceramides^{1c} do assemble to form amyloid like toxic structures and have implications in the etiology of rare inborn errors of metabolisms (IEMs) associated with these metabolite accumulation. In this context, our group for the very first time reported self-assembly of non aromatic amino acids like cysteine and methionine to amyloid-like cytotoxic structures.^{2a} Further we also reported unusual aggregates formed by other amino acids proline, hydroxyproline and lysine.^{2b} Our studies also suggested possible implications of these aggregates in the pathogenesis of IEMs like cystinuria, hypermethioninemia, prolinemia and lysinemia. Currently, we are studying the aggregation behavior of metabolites of urea cycle and uric acid pathways along with branched chain amino acids (BCAA) to investigate its relevance in diseases like Gout, Lesch-Nyhan Syndrome and Maple Syrup Urine Disease (MSUD).^{2c} In this talk, I will be presenting mainly the ongoing research on metabolite assemblies going in my lab, along with giving a brief overview of other related research.³

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- 1992-1997 Graduate Studies in Chemistry, University of Constance, Diplom,
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- 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
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Researcher-ID: [A-8498-2008](https://orcid.org/A-8498-2008)

1. Solid-Phase-Supported Chemoenzymatic Synthesis of a Light-Activatable tRNA Derivative A. Blümmler, H. Schwalbe,* A. Heckel,* *Angew. Chem. Int. Ed.* 2022, *61*, e202111613, DOI: [10.1002/anie.202111613](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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. Blümmler, A. Heckel,* H. Schwalbe,* *Angew. Chem. Int. Ed.* 2018, *57*, 12017–12021, DOI: [10.1002/anie.201807125](https://doi.org/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](https://doi.org/10.1038/s41467-018-03375-w)
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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]

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Probing nucleic acid conformations using responsive nucleoside probes

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Numerous biophysical tools have provided efficient systems to study nucleic acids. However, our current understanding on how nucleic acid structure complements its function, particularly in cellular environment, is limited. This general limitation is largely due to the lack of probes that can be used in both cell-free and cellular assays, and in more than one biophysical technique. Hence, correlating the information obtained under equilibrium conditions, in solid state and in cells becomes very difficult using uniquely-labeled oligonucleotide sequences. In this context, moving away from the tradition approach of “one label one technique” we adopted an innovative approach to investigate the nucleic acid structure and function in cell-free and cellular environments by using conformation-sensitive multifunctional nucleoside analog probes. Based on this strategy, we developed nucleoside analogs equipped with two or more labels (eg., fluorophore, NMR isotope label and X-ray crystallography phasing atom), which serve as common probes for analyzing nucleic acid motifs simultaneously by using a combination of fluorescence, NMR and X-ray crystallography techniques.¹⁻³ In parallel, we also develop chemo-enzymatic labeling technologies to functionalize and image nucleic acids *in vitro* and live cells.^{4,5} In this presentation, I will discuss the utility of our nucleoside probes and clickable nucleoside analogs in investigating nucleic acid conformations, recognition and function.

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Molecular Theranostics

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Over a decade of research has positioned theranostics (diagnostic therapy) as promising and integrated approach to advance biomedicine. The term theranostics essentially conveys the idea of combining therapeutic and diagnostic modalities to provide a holistic solution for disease management, including assessment of disease staging, treatment planning, and therapeutic efficacy. Generally, radiopharmaceutical, nano and macromolecular systems have been employed as theranostic tools to manage disease progression and cure. In recent years, the field has witnessed the emergence of small molecules or small molecular conjugates as theranostic tools. In this talk, I shall present our efforts towards the development of small molecular tools targeting canonical and noncanonical nucleic acids to image and ameliorate the pathological conditions.

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