

A Report on Four-day Virtual International Conference on
“ChemConvergence2025: Advancing Chemistry Through Multidisciplinary Innovations”
 Organized by **Department of Chemistry**
 in association with **The Indian Photobiology Society**
 from **04.03.2025 to 07.03.2025**



Report Submitted by: Dr. Rashmi Roy, Assistant Professor, Department of Chemistry.

Resource persons Details: Prof. Y. D. Vankar (retired professor IIT Kanpur), Prof. Lutz Ackermann (Professor Director Woehler Research Institute for Sustainable Chemistry, Georg-August- Universitaet Goettingen, Germany), Dr. Asif Iqbal (Assistant Professor, Kanazawa University Japan), Prof. Alakesh Bisai (Professor, IISER Kolkata, Council member Indian Photobiology Society), Dr. Partha Pratim Pal (Deputy Editor ‘Chemistry: An Asian Journal’, deputy editor of ‘Physical Sciences Journal’ Wiley-VCH), Dr. Manav Saxena (Associate Professor, Jain University, Bangalore), Dr. Nishamol Kuriakose (Postdoc, Univ. of Oslo, Norway), Dr. Supriya Dey (Harvard University, USA), Dr. Jhimli Bhattacharya (HOD, Associate Professor, NIT Nagaland), Prof. Pratim Kumar Chattaraj (Distinguished Prof., BITS Mesra, retired from IIT Kharagpur), Dr. Abhijit Bijanu (Assistant Professor, MITS, Madanapalle), Prof. Shoubhik Das (University of Bayreuth, Germany), Dr. Subrata Patra (Postdoc, Univ. of Bern, Switzerland), Dr. Harikrishna Sahu (Research Scientist II, Georgia Tech University, USA), Dr. Naganabonia Vijaykumar (Head, Process R & D, Wanbury Ltd.), Prof. Manabendra Sarma (Professor, IIT Guwahati), Prof. Abhijit Patra (Professor, IISER, Bhopal), Dr. Raj Sharma (Director, Aurigene Pharmaceutical Services, Hyderabad), Dr. Uttam Dhawa (Postdoc, EPFL, Switzerland), Dr. Moushumi Sarma (Principal Research Scientist, University of Kentucky, USA), Dr. Indrajit Paul (Postdoc, UCLA, USA), Dr. Aditi Agarwal (Principal Consultant, Infosys), Dr. Prantik Maiti (Group Leader, TCG Lifesciences), Dr. Sanoop P. (Assistant Professor, Dept. of Chemistry, MITS, Madanapalle), Dr. Rashmi Roy (Assistant Professor, Dept. of Chemistry, MITS, Madanapalle).

Attendees: More than 100 participants registered (National & International) from the USA, Switzerland, France, Norway, and India. 50 poster presentations took place throughout the 4 days. 25 invited speakers from India and abroad delivered lectures in this conference.

Mode of Conduct: Online

Report Received on 18.03.2025.

Advisory Committee:

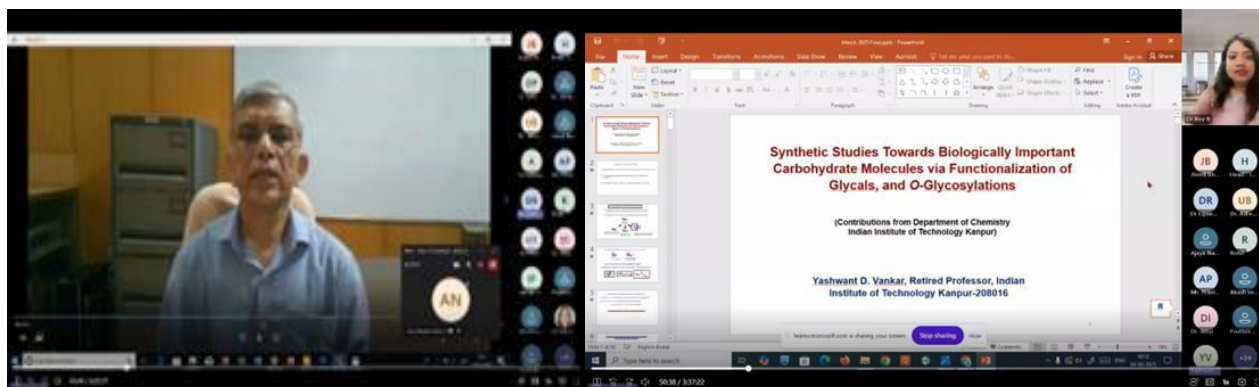
Prof. Ashok Kumar Mishra (IIT Madras, President Indian Photobiology Society), **Prof. Chittaranjan Sinha** (retired professor from Jadavpur University, Secretary, Indian Photobiology Society), **Prof. Alakesh Bisai** (Professor, IISER Kolkata, Council member-Indian Photobiology Society), **Dr. Satyajit Saha** (Assistant Professor, ICT Mumbai), **Dr. Raj Sharma** (Director, Aurigene Pharmaceutical Ltd.), **Dr. Raghu Chitta** (Associate Professor, NIT Warangal)

Day-1 (04/03/2025)

The Department of Chemistry at Madanapalle Institute of Technology & Science, Madanapalle, organized a ‘Four Day Virtual International Conference’ entitled “ChemConvergence2025: Advancing Chemistry Through Multidisciplinary Innovations” during 4th-7th March 2025. The Inauguration program was started at 9:30 AM by Dr. **Lipeeka Rout** (Asst. Prof. Dept. of Chemistry, MITS), who invited the convener Dr. **Rashmi Roy** to deliver a welcome address to the respected dignitaries, distinguished delegates, and all the participants. Then, **Dr. Renjith Bhaskaran** (HOD, Chemistry Dept.) gave the Inaugural welcome address to all the dignitaries, delegates, and participants. In addition, Dr. **P. Ramanathan** (Vice Principal Academics- MITS, Madanapalle) also gave the inaugural address to the gathering virtually. Afterward, the

president of the Indian Photobiology Society, Professor Ashok Kumar Mishra (IIT Madras), gave a welcome address to all the delegates and participants virtually.

The first session of Day-1 talk started at 10.10 AM chaired by Dr. Lipika Rout (Asst. Prof., Dept. of Chemistry, MITS) who introduced the resource person of plenary lecture-I Prof. Y. D. Vankar (Retired Professor, IIT Kanpur, Uttar Pradesh), to the participants and thanked him for accepting the invitation. Further, the academic profile of Prof. Y. D. Vankar was being introduced to the gatherings by the chair through a virtual mode.



Prof. Y. D. Vankar began the lecture by sincerely thanking the audience, the Convener Dr. Rashmi Roy, HOD Chemistry, the Principal, the Vice Principal, and the Management of MITS Madanapalle for providing him with the chance to share his expertise in chemical science research and related fields. The title of the talk was “**Synthetic Studies Towards Biologically Important Carbohydrate Molecules via Functionalizing of Glycals, and O-Glycosylations**”. He discussed how during the past 3 decades, his group entered the arena of Synthetic Carbohydrate Chemistry involving (i) C-2 functionalization of glycals, and (ii) newer methods for O-glycosylations. Applications of these synthetic methods were presented for the synthesis of some biologically important molecules such as glycosidase inhibitors and trisaccharide. Finally, he answered all the questions raised by the audience.

The second talk of the session began at 11.00 AM and the resource person was introduced by Dr. Lipika Rout who gave a brief introduction about the resource person Dr. Asif Iqbal (Assistant Professor, Kanazawa University Japan). Dr. Asif Iqbal’s academic profile was being introduced to the participants by the session chair.



In his opening remarks, Dr. Asif Iqbal expressed his gratitude to the audience, the organizers, the Convener Dr. Rashmi Roy, the HOD, the Principal, the Vice Principal, and the Management of MITS Madanapalle for allowing him to share his knowledge of chemical science research and associated subjects. The title of his talk was “**Stimuli-responsive helicity inversion speed control in dynamic helical trinickel(II) metallocryptand**”. During his talk, he spoke about the

development of artificial dynamic helical molecules with controllable helix inversion rate that can be useful to make chiral memory materials.¹ Most of the previous reports of stimuli-responsive chiral molecules have been focused only on the equilibrium states before and after stimulation but not on controlling the kinetics.¹ We have already demonstrated that the helicity inversion kinetics of trinickel(II) cryptands can be controlled by guest recognition in the cryptand cavity.² Here, we present that the chirality inversion kinetics of a trinickel(II) cryptand can be controlled by guest recognition in the cryptand cavity.³

When the guest was absent, the nickel (II) cryptand underwent a dynamic interconversion between the *P* and *M* forms in solution, preferring the *M* form, with a half-life of $t_{1/2} = 4.99$ min. The *P/M* equilibrium is reversed to *P*-favored state by binding with an alkali metal ion in the cryptand cavity. The timescale of this *M*→*P* inversion kinetics was both notably accelerated and decelerated by the guest binding ($t_{1/2} = 0.182$ min for K^+ complex; 186 min for Cs^+ complex); thus, the equilibration rate constants differed by up to 1000-fold depending on the guest metal ions. This acceleration/deceleration can be explained in terms of the virtual binding constants at the transition state of the *P/M* chirality inversion; K^+ binding more stabilizes the transition state rather than the *P* and *M* forms to result in the acceleration.

Dr. Rahul Pal, assistant professor of chemistry at MITS, presided over the first talk of the second session (Day I). On Day-I, the first talk of the session-II began at 11.50 AM. He welcomed Dr. Partha Pratim Pal (Deputy Editor ‘Chemistry: An Asian Journal’, deputy editor of ‘Physical Sciences Journal’ Wiley-VCH) and thanked him for accepting the invitation. Additionally, Dr. Rahul Pal introduced Dr. Partha Pratim Pal’s academic background to the participants.

In his opening remarks, Dr. Partha Pratim Pal expressed his gratitude to the audience, the organizers, the Convener, the Principal, the Vice Principal, and the Administration of MITS Madanapalle for allowing him to impart his knowledge in journal publishing. The title of his talk was “**Editorial Tips for Successful Publishing**”. He discussed that navigating the road from laboratory results to publishing them in a prestigious journal is an important aspect of a researcher’s life. Insights from the editorial desk can improve an author’s understanding of the publishing process, which in turn should increase their chances of publishing in high-impact journals. In this talk, he mainly focused on providing editorial tips for successfully bringing research from the laboratory to a journal. Some of the questions he addressed are the role of an editor, core principles of the peer-review process, publishing ethics, open science and the role of AI/ML in the publishing industry. Finally, he addressed the participants’ questions.

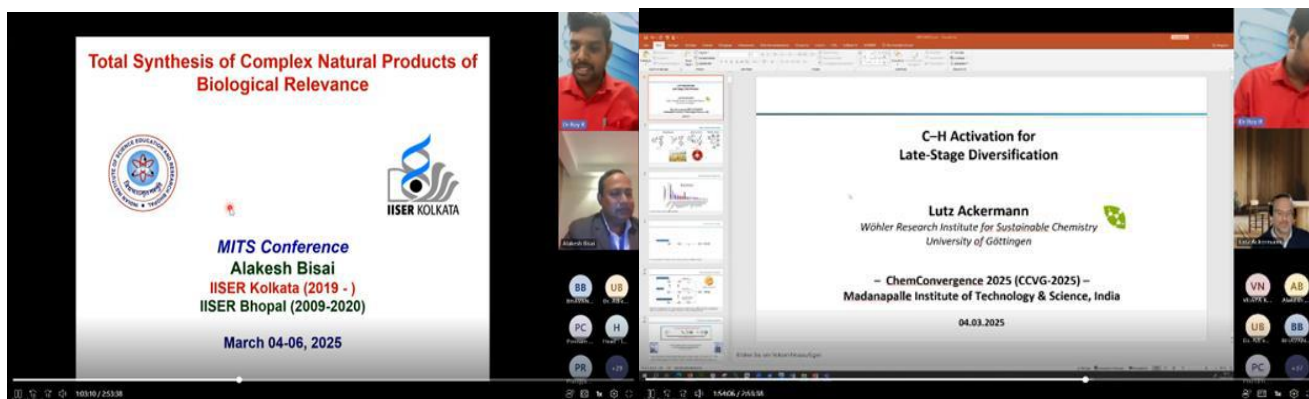
The second talk of Session II (Day-I) began at 12.40 AM and the resource person was introduced by the session chair Dr. Rahul Pal, who gave a brief introduction about the resource person, Dr. Manav Saxena (Associate Professor, Jain University, Bangalore). Dr. Rahul Pal introduced Dr. Manav Saxena’s academic background to the participants virtually.



Dr. Manav Saxena thanked everyone for the opportunity to speak about chemical catalysis research and its industrial perspective, including the audience, the convener, the organizers, the HOD Chemistry, the Principal, the Vice Principal, and the Management of MITS Madanapalle. The title of the talk was “**Ultrathin 2D Nickel/Cobalt Hydroxide Vertical Heterostructures: Unlocking High Energy Density for Flexible Symmetric Solid-State Micro-supercapacitor**”. His topic of discussion covers the following concepts. Assembling 2D ultrathin nanosheets into vertical heterostructures offers significant potential for advanced energy storage due to enhanced active sites, improved ion diffusion, and increased electrical conductivity, leading to superior ion/electron transport, higher energy density, and improved rate performance. However, breaking crystal symmetry and fostering the anisotropy in crystal growth is critical in non-layered materials. Overcoming challenges such as random assembly, complex synthesis, instability, and poor interfacial contact is critical. This study synthesizes 2D Nickel/Cobalt hydroxide vertical heterostructures (nickel as the top layer) using a wet chemical process, achieving 32% higher areal charge storage compared to cobalt/nickel hydroxide and 57% and 330% better than individual Ni(OH)₂ and Co(OH)₂. The synergistic interaction between nickel and cobalt hydroxides contributes to a high volumetric capacity (710 mAh cm⁻³) and energy density (285 mWh cm⁻³) in symmetric devices. The flexible micro-supercapacitor retains 75% capacitance after 15,000 cycles and demonstrates stability under bending up to 135°, with a volumetric capacity of 393 mAh cm⁻³. DFT simulations complement experiments, revealing interaction energy and electronic state redistribution near the Fermi level. This integrated approach serves as a guide for enhancing electrochemical properties in 2D heterostructures, aiding in the development of next-generation, high-performance energy storage materials.

After the end of the second session (Day 1), **Professor Chittaranjan Sinha (Jadavpur University, Secretary, Indian Photobiology Society)** addressed the virtual audience. The convener of the conference, **Dr. Rashmi Roy**, gave a brief academic background of Prof. Chittaranjan Sinha. **Prof. Chittaranjan Sinha** gave a virtual talk regarding the collaboration between ‘MITS Madanapalle’ and ‘The Indian Photobiology Society’. He gave a detailed description of the activities of the ‘**Indian Photobiology Society**’.

The opening presentation of the third session (Day-I) was led by Dr. **Rajaram R.** (Asst. Prof, Dept. of chemistry, MITS) at 2.00 PM. Professor Alakesh Bisai (**Professor, IISER Kolkata**) in India was requested to deliver her talk, and he was welcomed and thanks for accepting our invitation. The participants were also given an overview of Prof. Alakesh Bisai’s academic history by Dr. Rajaram R.



Dr. Alakesh Bisai thanked the audience, the convener, the head of the chemistry department, the principal, the vice principal, and the administration of MITS Madanapalle for allowing him the chance to share his expertise in chemical science research

and related fields. "Natural Products of Biological Relevance: Learning from Nature" was the title of his speech. He mainly covers synthesis of atropo-diastereomers as synthesized in his lab. The natural product chemical diversity is more closely aligned with drugs than synthetic libraries, thus making them ideal candidates for drug discovery projects.¹ Marine organisms can be considered the most recent source of bioactive natural products in relation to terrestrial plants and nonmarine microorganisms.² The beauty of Nature is that she produces a variety of complex natural products in entioenriched form.³⁻⁴ In the above context, naturally occurring alkaloids with impressive diversity of biological activities drew our interest for the development of bio-inspired strategies. ⁵⁻⁶ Towards this, we explored novel strategies that will be discussed in this talk.

The resource person of the **plenary lecture** of Session III (Day-I) was Professor **Lutz Ackermann**. He was introduced by Dr. Rajaram R. who gave a brief introduction about **Professor Lutz Ackermann (Professor Director Woehler Research Institute for Sustainable Chemistry, Georg-August- Universitaet Goettingen, Germany)**. The session began at 2.45 PM. **Professor Lutz Ackermann** thanked everyone for the opportunity to speak about chemical science research and related topics, including the audience, the convener, the HOD Chemistry, the Principal, the Vice Principal, and the Management of MITS Madanapalle. The title of his talk was "**Catalyzed C–H Functionalization**". He discussed the current study being conducted by his research team during his presentation, which focused on the different chemical strategies for effective C-H activation. C–H activation has surfaced as a powerful platform in molecular synthesis, with transformative applications to material sciences and drug discovery, among others. In this context, we have introduced carboxylates, for position-selective C–H activation with versatile ruthenium (II) complexes. In light of limited resources, we developed Earth-abundant 3d metal catalysis based on detailed mechanistic insights. Studies towards metallaelectrocatalytic C– H and C–C activation with a unique level of resource-economy, late-stage functionalization, data science, and enantioselective catalysis will be discussed, with a topical focus on sustainable base metals.

The resource person of the 3rd invited talk of Session III (Day-I) was **Dr. Nishamol Kuriakose (Postdoc, Univ. of Oslo, Norway)**. Dr. Rajaram R. gave a brief introduction of **Dr. Nishamol Kuriakose**. The session began at 3.25 PM. The title of her talk was "**Feature engineering and machine learning-based prediction of hydrogen adsorption for MOF materials**". In her study, she applied machine learning models to identify MOF materials with high hydrogen adsorption capacity at room temperature. Accurate MOF descriptors, representing both geometry and chemistry, are crucial for such studies. For geometric representation, they used simple descriptors like pore size, volume, and surface area. To capture MOF chemistry, they extended the AABBA vectors—a graph kernel originally.



used to predict chemical properties of transition-metal complexes—into our MOF models. These AABBA descriptors, derived from the crystallographic information files (CIFs), incorporating edge-based features of a MOF based on xTB calculations, provide an enhanced representation of MOF chemistry, enabling the prediction of hydrogen adsorption capacities.

At the end of day-I, the virtual poster presentation was conducted which began at 3.45 PM. There were a totally 14 participants who presented their posters on Day-I. Each participant presented their poster for around 8 mins duration, and judges asked questions for around 2 mins to evaluate the posters. Poster presentation was completed around 7.00 PM. The first day of the conference concluded at 7.10 PM with a few announcements made by the convener, Dr. Rashmi Roy.

Day-2 (05/04/2025)

Convener Dr. Rashmi Roy began the program on Day 2 at 9.40 AM by welcoming the participants with a few announcements about the CCVG-2025 conference. The first session of the Day-II talk began at 9:50 AM, and Dr. Ugrabadi Sahoo, an assistant professor of chemistry at MITS, presided. He welcomed the attendees and thanked Dr. **Supriya Dey (Harvard University, USA)**. Dr. Supriya Dey's academic background was also presented in front of the gathering virtually.

Year	Research Group	Synthetic steps and yield	Stereoselective Glycosylation?
2013	Lin	>36 steps, 0.017%	No
2014	Wang	64 steps and 0.02%	No
2014	Hung	36 steps, 0.063%	Some cases
2017	Wang	45 steps, 1%	No

Doses and price

- Fondaparinux is administered by deep subcutaneous injection
- The recommended dose of fondaparinux is 7.5 mg (patients with body weight ≥ 50 , ≤ 100 kg) once daily
- 7.5mg/4.6ml - \$166-200
- Source: Only Chemical Synthesis

Solution/Our Approach

- Programmable one-pot synthesis
- α -selective glycosylation influenced by the TBDPS & OAc at O-6 position
- 3.5% overall yield
- 24 steps for lowest linear route

In his opening remarks, Dr. Supriya Dey expressed his gratitude to the audience, the convener Dr. Rashmi Roy, the HOD Chemistry, the Principal, the Vice Principal, and the Management of MITS Madanapalle for allowing him to impart his knowledge in chemical science research and associated fields. He delivered a talk on “**Programmable One-Pot Synthesis of Heparin Sulfate and Heparin-derived Commercial Anticoagulants**”. The theme of Dr. Supriya Dey’s talk was based on synthetic carbohydrate chemistry. The development of efficient synthetic methods of heparin sulfate and heparin-derived commercial anticoagulants are important from the standpoint of understanding different biological processes, understanding its potential for drug discovery and to cope with the current market demand and cost of commercial anticoagulants. The synthesis of heparin sulfate and anticoagulants (Fondaparinux & Idraparinux) is very challenging due to the difficulty in the regio- and stereoselective glycosylation and the strategic installation of OSO₃ and NHSO₃ groups. We have developed a computer program, namely, AUTO-CHO, based on the concept of quantitative determination of the relative reactivity values (RRV) of a thioglycoside donor for the synthesis of heparin sulfate and commercial anticoagulants with improvement in both in terms of synthetic steps and yield. In this talk, I will discuss the development of AUTO-CHO software and its application in complex oligosaccharide synthesis.

The second talk of the session I started at 10.30 AM, and the resource person was Dr. **Jhimli Bhattacharya**, an **associate professor** in the department of chemistry at **NIT Nagaland** in India. **Dr. Jhimli Bhattacharya** was introduced by Dr. Ugrabadi Sahoo, and he used virtual reality to introduce her academic background to the participants.

For the opportunity to talk about chemical science research and related topics, Dr. Jhimli Bhattacharya thanked the audience, the Convener Dr. Rashmi Roy, the HOD Chemistry, the Principal, the Vice Principal, and the Management of MITS Madanapalle. The topic of the presentation was “**On Plant Alkaloids Derived from Northeast Indian Biodiversity: An Ethnomedical and Biophysical Approach.**” She delivered a talk about the plant alkaloids from Northeast India. North-Eastern (NE) India is known for its diverse biodiversity which is enriched with various unique medicinal plants. Healthy lifestyle and the traditional medicines (ethno-medicines; derived from the local medicinal plants) are integral part of the ethnic, indigenous tribal societies. The rich biodiversity ensures tremendous potential of such several ethnomedicines which are well known for their natural healing power. In this study we have reviewed some of the important indigenous medicinal plants from Nagaland (one of the most important states of NE India) and the results are analyzed from ethno botanic point of view. A detailed survey work was carried out involving the local Naga population and medical practitioners (“Koviras”) relating to the plants/parts used by the localities for the medicinal purpose. Special emphasis was given to identify the exact part of the plants (stem, leaves, bark, root, fruit, flower etc.) that are used as natural remedies. Hence, the active ingredients/chemical compounds responsible for the medicinal properties were identified with the help of a literature review. In most of the cases, it was found that the alkaloids and flavonoids present in the different parts of the plants are responsible for their medicinal properties.

Though traditional medicines from plant origins are quite popular here, the scientific background of the effectiveness of these natural drugs and their mechanism of action are yet unexplored. Thus, the next part of the study was focused on a few plant-derived alkaloids that have maximum usage in Nagaland.

The second session (Day II) was chaired by Dr. Sanoop P., an assistant professor of chemistry at MITS. The first talk of the second session of Day II was a plenary lecture by **Prof. Pratim Kumar Chattaraj (Distinguished professor, BITS Mesra)**. His plenary lecture began at 11.30 AM. **Prof. Dr. Pratim Kumar Chattaraj** was welcomed and thanked for accepting the invitation. Dr. Sanoop P. also gave the participants an overview of **Prof. Pratim Kumar Chattaraj**’s academic background.

Aromaticity and Conceptual DFT

Prof. P. K. Chattaraj
Department of Chemistry
Indian Institute of Technology
Kharagpur - 721 302, India

MITS MADANAPALLE **CSIR-AMPRI** **AcSIR**

Lead-free, Flexible, and Lightweight, Metal-Polymer Composite for Ionizing Radiation Shielding Application

4-day Virtual International Conference on ChemConvergence 2025
In association with Indian Photobiology Society

Dr. Abhijit Bijanu
Assistant Professor, MITS
Madanapalle Institute of Technology and Science, Madanapalle, Andhra Pradesh, 517325, India

Prof. Pratim Kumar Chattaraj thanked the MITS Madanapalle administration, the audience, the organizers, the Principal, and the Vice Principal for the opportunity to share his expertise in chemical science research and related fields. "**All-metal aromaticity and Hydrogen storage**" was the topic of his talk. His lecture was based on the following topic. Several metal clusters exhibit aromatic behavior. Conceptual density functional theory has been found to be useful in analyzing the behavior of all-metal aromatic compounds like and all-metal antiaromatic compounds like and their complexes in terms of different global and local reactivity descriptors as well as the nucleus independent chemical shift. Aromaticity and antiaromaticity in cyclic alkali clusters like and , polyacene analogues of inorganic ring compounds, multivalent superatoms, trigonal cyclic -bonded dianions like and as well as their different sandwich and multi-decker complexes are analyzed in terms of those reactivity descriptors and the associated electronic structure principles. The hydrogen storage ability of these clusters has been explored.

The second talk of Session II (Day-II) began at 12.20 AM, and the resource person was introduced by Dr. Sanoop P., who gave a brief introduction about the resource person Dr. Abhijit Bijanu (Assistant Professor, Department of Chemistry, MITS, Madanapalle).

For the chance to discuss chemical science research and related topics, Dr. Abhijit Bijanu expressed his gratitude to the audience, the lecture's organizers, the Principal, the Vice Principal, and the Management of MITS Madanapalle. His talk was titled "**Lead-free, Flexible and Lightweight, Metal-Polymer Composite for Ionizing Radiation Shielding Application**". His talk was based on the following topic.

Ionizing radiation is hazardous for human beings. In today's world radiation is used in several fields like diagnostic imaging, medicinal industries, etc. Hence, radiation-shielding materials are in high demand. Conventionally, lead and lead-based materials are used for shielding ionizing radiation due to its high density and high atomic number². But lead is one of the most toxic and hazardous substances, and lead-based X-ray shielding apparel has been of great concern in recent years due to its rigidity, high toxicity, and heavy weight, thus making it uncomfortable during use. So, researchers are looking for an alternative to lead-based material. High Z non-toxic metal/metal compound incorporated polymer composite materials have gained a lot of attention in recent years.

The opening presentation of the third session (Day-II) was led by **Dr. Boobalan Ramadoss** (Asst. Prof, Dept. of chemistry, MITS) at 2.00 PM. **Prof. Shoubhik Das (University of Bayreuth, Germany)**, was requested to deliver his plenary lecture, and he was welcomed in the virtual conference. The participants were also given an overview of **Prof. Shoubhik Das's** academic history by **Dr. Boobalan Ramadoss**.

Prof. Shoubhik Das expressed his gratitude to the audience, the organizers, the principal, the vice principal, and the MITS Madanapalle administration, allowing him to share his knowledge of chemical science research and associated subjects. His talk was entitled "**Photocatalysis as a green tool for the development of sustainable chemistry.**" His lecture was based on the following topic. Recently, solar energy has exhibited great potential as a promising alternative to traditional energy sources because it is renewable, abundant, affordable, and everlasting. Among various solar energy conversion techniques, photocatalysis is deemed a promising, environmentally benign, and cost-effective strategy to generate both fuels and high-value chemicals. While in this domain, homogeneous photocatalysts prevail due to higher selectivity, but the reutilisation of the catalyst is next to impossible. On the other hand, heterogeneous photocatalysts are recyclable but not highly selective. Therefore, to make a bridge between these two, a new strategy has been developed by synthesizing single metal atom photocatalysts that are selective as well as recyclable.

The resource person of the second talk of Session III (Day-II) was introduced by **Dr. Boobalan Ramadoss**, who gave a brief introduction about the resource person, **Dr. Subrata Patra (Postdoctoral Fellow, University of Bern, Switzerland)**. The session began at 3.00 PM.

Dr. Subrata Patra thanked everyone for the opportunity to speak about chemical science research and related topics, including the audience, the Convener Dr. Rashmi Roy, the HOD of Chemistry, the Principal, the Vice Principal, and the Management of MITS Madanapalle. His title of the talk was "**Facile Access to Terminal Nitroalkanes via Anti-Markovnikov Nitration and Nitroalkylation Enabled by Photoredox Catalysis**". He discussed about the following investigations done in their postdoctoral lab.

The nitro group (NO₂) is essential in organic synthesis, but nitration remains challenging due to limitations of traditional methods, which rely on corrosive acid mixtures and are unsuitable for acid-sensitive compounds. This highlights the need for safer, selective nitration protocols under mild conditions. They reported the first intermolecular anti-Markovnikov hydronitration of alkenes using visible light-mediated photoredox catalysis. Utilizing N-nitrosuccinimide as a redox-active nitrating reagent, nitryl radicals undergo regioselective addition with olefins and a hydrogen atom transfer (HAT) mediator, producing terminal nitroalkanes. This system also enables chain expansion via anti-Markovnikov addition with substituted

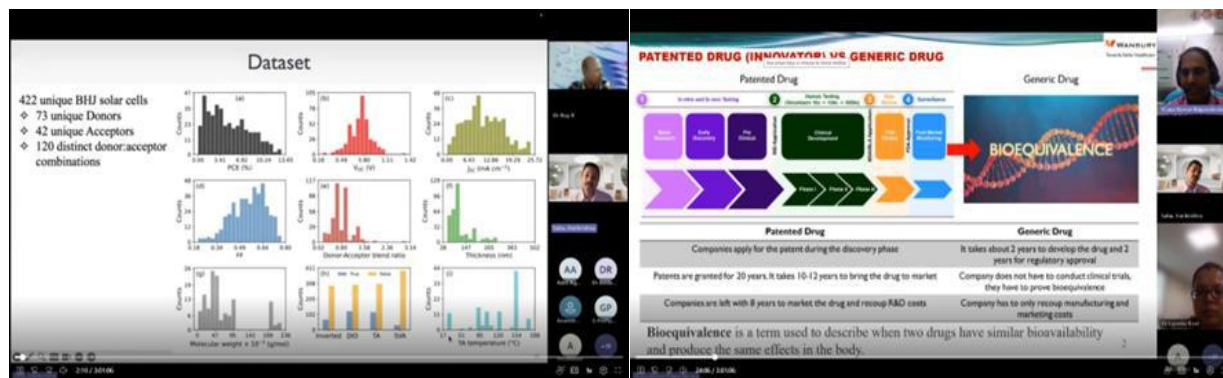
bromonitroalkanes. These transformations provide a safe, efficient route to nitro-functionalized compounds, addressing key challenges in nitration chemistry. Finally, he explained in detail the quarries of the participants.

The virtual poster presentation of 'Day-II' started at 3.30 PM. On Day II, 15 contestants in all displayed their posters. Each competitor gave a presentation of their poster for around 8 minutes, and then the judges took questions for 2 mins to determine the best posters. Around 7.10 PM, the poster presentation was finished. At 7.15 PM, the conference second day came to an end with a few announcements from the convener, **Dr. Rashmi Roy**.

Day-3 (06/08/2024)

On Day 3, at 9.30 AM, **Convener Dr. Rashmi Roy** welcomed the participants and made a few announcements regarding the 'CCVG-2025' conference. At 9.40 AM, **Dr. Amaladass P.**, an assistant professor of chemistry at MITS, presided over the opening session of the Day-III discussion. He greeted the audience and expressed gratitude to **Dr. Harikrishna Sahu (Research Scientist II, Georgia Tech University, USA)** for becoming an invited speaker for the **virtual international conference CCVG-2025**. **Dr. Amaladass P.** also provided the audience with an overview of **Dr. Harikrishna Sahu's** academic background through virtual presentations.

In his opening remarks, **Dr. Harikrishna Sahu** expressed his gratitude to the audience, the organizers, the Principal, the Vice Principal, and the Management of MITS Madanapalle for allowing him to impart his knowledge in chemical science research and associated fields. He delivered a talk on "**From Corpus to Innovation: Accelerating Organic Photovoltaic Discovery Using Large Language Models**". The topic of his discussion is portrayed below. Traditional methods for materials discovery, relying on experimental trials, computational simulations, and heuristics, are time-consuming, resource-intensive, and limited in scope. Despite the increased use of machine learning (ML), conventional approaches face two key challenges: (1) the availability of informatics-ready data and (2) the complexity of numerical descriptors. Scientific knowledge on materials is scattered across numerous publications, databases, and supplementary materials, making comprehensive data collection daunting and error-prone. This work presents a novel framework leveraging TinyLlama-1.1B, a large language model (LLM)-driven framework to accelerate OPV materials discovery by extracting structured data from scientific literature and predicting device performance using natural language embeddings. Finally, he addressed the participants' queries.



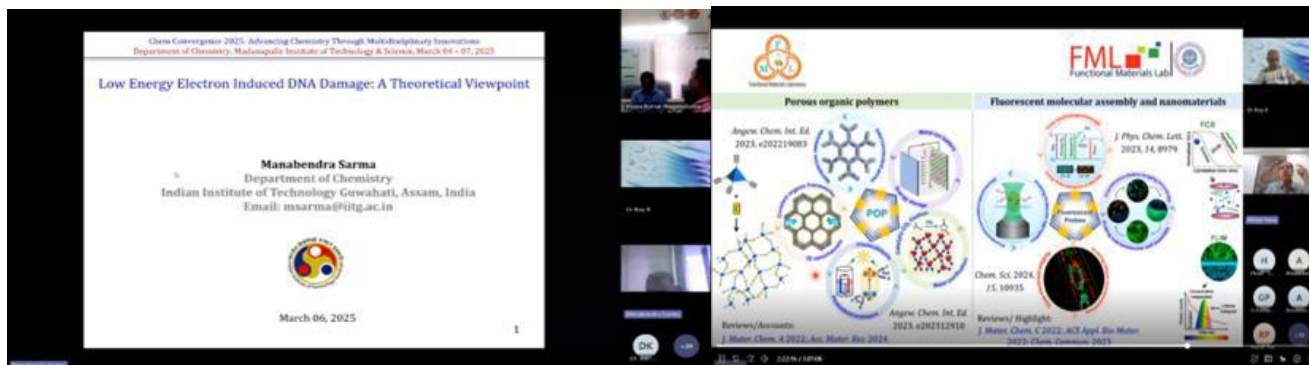
The second talk of the 1st session started at 10.40 AM. **Dr. Amaladass P.** introduced the invited speaker **Dr. Naganabonia Vijaykumar (Head, Process R & D, Wanbury Ltd.)** & gave a brief account of his academic accomplishments to the participants.

For the opportunity to talk about chemical science research and related topics, **Dr. Naganabonia Vijaykumar** thanked the audience, the convener **Dr. Rashmi Roy**, the organizers, the HOD Chemistry, the Principal, the Vice Principal, and the Management of MITS Madanapalle. The topic of the presentation was "**Transforming API Process Development with AI and Quality by Design (QbD): A Multidisciplinary Approach**". His talk includes **real-world case studies** demonstrating how **pharmaceutical companies** are leveraging **AI-based predictive analytics and process optimization tools** to enhance API development. The discussion also emphasizes the role of **cross-functional collaboration between chemists, data scientists, and engineers** in driving the next wave of **multidisciplinary innovation in pharmaceutical manufacturing**.

The opening lecture of the second session (Day-III) was presided over by **Dr. Ragavendran K.** (Assistant Professor, MITS). The session began at 11.10 AM with a plenary lecture by **Professor Manabendra Sarma** (Professor of chemistry at **IIT Guwahati, India**). Professor Sarma was welcomed and thanked for accepting the invitation by the session chair. The chair also gave the academic background of the speaker to the participants.

Professor Manabendra Sarma expressed his gratitude to the MITS Madanapalle administration, the attendees, the lecture's organizers, the HOD Chemistry, the Principal, and the Vice Principal for the chance to present his knowledge in chemical science research and associated fields. His lecture was entitled "**Low Energy Electron Induced DNA Damage: A Theoretical Viewpoint**." He discussed the following topic. In radiotherapy, the interaction between ionizing radiations and the surrounding aqueous medium in the body produces many secondary species, such as low-energy electrons (LEEs), cations, and free radicals. The LEEs attach to the nucleobases very quickly in their π^* orbitals, which can lead to various types DNA damage, i.e., double-strand breaks, single-strand breaks, nucleobase release, and other clustered damage. Prof. Sarma's group studied dissociative electron attachment (DEA) pathways using electronic structure calculations and the time-dependent wave-packet approach. They focused on base release (C-N bond rupture) and single-strand rupture processes. In the 2'-deoxycytidine-3'-monophosphate (3'-dCMPH) moiety, it was observed that base release occurs at relatively higher energy compared to strand breaks. Additionally, they studied 2'-deoxycytidine-5'-monophosphate (5'-dCMPH), and it was observed

that the 5'C-O bond dissociation occurred in ~20 femtoseconds at an energy of 1 eV.5 We also investigated a sugar-phosphate-sugar (S-P-S) moiety.



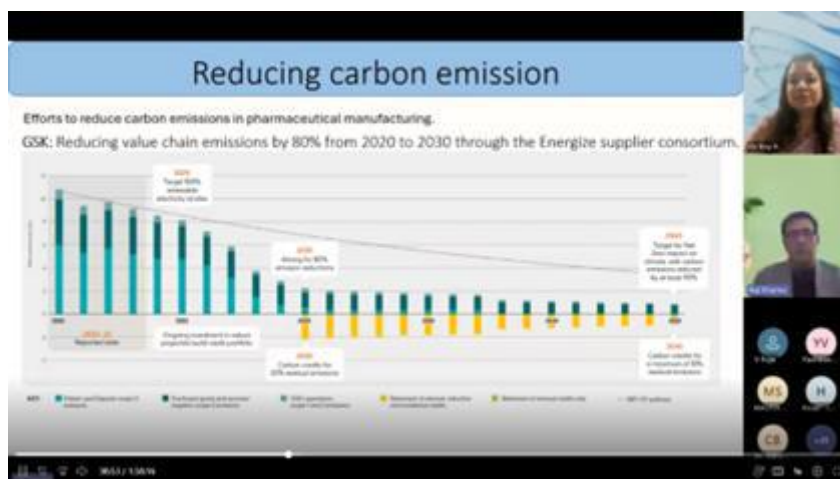
The second talk of Session II (Day-III) began at 12.20 AM, and the resource person was **Prof. Abhijit Patra (Professor, IISER Bhopal)**. Dr. Ragavendran K. chaired the session who gave a brief introduction about Professor Abhijit Patra, a life member of the '**Indian Photobiology Society**'. For the chance to discuss chemical science research and related topics, **Professor Abhijit Patra** expressed his gratitude to the audience, the convener Dr. Rashmi Roy, the HOD Chemistry, the Principal, the Vice Principal, and the Management of MITS Madanapalle. His talk was titled "**Nanoporous Organic Materials for Energy and Environmental Sustainability.**" He discussed the following topic.

The interfacial polymerization developing processable nanoporous organic thin films of crystalline covalent organic frameworks (COFs) could be promising for applications from molecular separation to energy storage. In this context, Prof. Patra's group achieved a room-temperature transformation of an organic imine cage to a free-standing COF film at the aqueous-organic interface using an amine linker exchange strategy, producing highly porous and crystalline COF films in 24 h. The COF film showed high permeance and excellent molecular sieving performance. Additionally, a 2D electrochromic COF (EC-COF) film having tunable redox functionalities was developed at the solid-liquid interface with broad absorption across the UV-to-NIR range, showing three-state anodic electrochromism, high color contrast (~ 60 % in the NIR), and fast switching.

The opening presentation of the third session (Day-III) was led by **Dr. Rashmi Roy** (Asst. Prof, Dept. of chemistry, MITS and the convener, CCVG-2025) at 2.00 PM. **Dr. Raj Sharma (Director, Europe Business Development, Aurigene Pharmaceutical Services)** was requested to deliver his talk, and he was welcomed and thanked for accepting our invitation. The participants were also given an overview of Dr. Raj Sharma's academic history by Dr. Rashmi Roy. Dr. Sharma thanked everyone for the opportunity to speak about chemical science research and related topics, including the audience, the convener Dr. Rashmi Roy, the HOD Chemistry, the Principal, the Vice Principal, and the Management of MITS Madanapalle. The title of his talk was "**Innovative Pathways to Sustainable Development and Manufacturing in the Pharmaceutical Industry**". Dr. Raj Sharma discussed the following topics in his lecture.

The pharmaceutical industry is increasingly focusing on sustainable development and manufacturing practices to address environmental, economic, and social challenges. Currently, pharma companies are exploring innovative pathways to achieve sustainability in manufacturing, emphasizing the integration of eco-friendly processes, waste reduction, and the adoption of Industry 4.0 technologies. Recent advancements and case studies highlight the benefits and challenges associated with sustainable practices in the pharmaceutical sector. Sustainable manufacturing not only enhances environmental performance but also improves operational efficiency and regulatory compliance, paving the way for a more resilient and responsible pharmaceutical industry. Finally, he successfully explained all the questions that arose from the audience.

The resource person of the second talk of Session III (Day-III) was introduced by **Dr. Boobalan Ramadoss** (Assistant Professor, Dept. of Chemistry, MITS), who gave a brief introduction about the resource person **Dr. Uttam Dhawa (Postdoc, EPFL, Switzerland)**. The session began at 2.40 PM. Dr. Boobalan Ramadoss introduced Dr. Uttam Dhawa's academic background to the participants through online mode.



Dr. Uttam Dhawa thanked everyone for the opportunity to speak about chemical science research and related topics, including the audience, the organizers, Dr. Rashmi Roy, the HOD Chemistry, the Principal, the Vice Principal, and the

Management of MITS Madanapalle. The title of his talk was “*Nickel-Catalyzed Enantio- and Diastereoselective Synthesis of Fluorine-Containing Vicinal Stereogenic Centers.*” He discussed the following topic.

The construction of fluorinated architectures has been a topic of interest to medicinal chemists due to their unique ability to improve the pharmacokinetic properties of bioactive compounds. However, the stereoselective synthesis of fluoro-organic compounds with vicinal stereogenic centres is a challenge. Herein, they present a directing-group free nickel-hydride catalyzed hydroalkylation of fluoroalkenes to afford fluorinated motifs with two adjacent chiral centres in excellent yields and stereoselectivities. Their method provides expedient access to biologically relevant, highly enantioenriched organofluorine compounds. Furthermore, the strategy can be used for the diastereo- and enantioselective synthesis of vicinal difluorides, which have recently gained attention in the fields of organocatalysis and peptide mimics. Dr. Uttam Dhawa finally addressed the questions of the audience successfully.



The virtual poster session on Day III began at 3.15 PM. In the poster sessions, **15** contestants displayed their posters. Each competitor gave a presentation of their poster for around 8 minutes, and then the judges took questions for 2 minutes to determine which posters were the best. Around 6.30 PM, the poster presentation was finished. Dr. Rashmi Roy concluded the poster session at 6.40 PM of Day-III with a few important announcements.

Day-4 (07/03/2025)

On Day 4, at 9.30 AM, **Convener Dr. Rashmi Roy** welcomed the participants and delegates and made a few announcements regarding the ‘**CCVG-2025**’ conference. At 9.40 AM, **Dr. Rahul Pal**, an assistant professor of chemistry at MITS, presided over the opening session of the Day-IV discussion. He greeted the virtual audience and expressed gratitude to **Dr. Moushumi Sarma (Principal Research Scientist, University of Kentucky, USA)** for becoming an invited speaker for the **virtual international conference CCVG-2025**. **Dr. Rahul Pal** also provided the audience with an overview of **Dr. Moushumi Sarma’s** academic background through virtual presentations.



In his opening remarks, **Dr. Moushumi Sarma** expressed his gratitude to the audience, the organizers, the Principal, the Vice Principal, and the Management of MITS Madanapalle for allowing her to impart his knowledge in chemical science research and associated fields. She delivered a talk on “**Increasing CO₂ Capture Using Carbonic Anhydrase Mimics for Post-Combustion CO₂ Capture and Direct Air Capture**”. The topic of his discussion is portrayed below.

The rising concentration of carbon dioxide CO₂ greenhouse gas in the atmosphere is causing growing concern due to its potential adverse effects on the environment, leading to widespread attention. Using amine-based solutions for Post Combustion CO₂ capture in power plants is the most common method utilized industrially and studied in the laboratory environment. However, a limited number of amines are available for carbon capture research after balancing the capital cost and energy penalty. Direct air capture (DAC) is also becoming increasingly promising as numerous countries set goals to reduce CO₂ emissions. DAC technologies are designed to extract CO₂ directly from the atmosphere for storage or utilization purposes. One major obstacle facing DAC is the low concentration of CO₂, approximately 400 ppm, which necessitates processing large volumes of air to extract each mole of CO₂. In nature, the enzyme Carbonic Anhydrase is known to catalyze the reaction of CO₂ hydration. In this context, we have developed a series of metal complexes that can perform catalytic CO₂ hydration as a mimic of Carbonic Anhydrase, thereby increasing the CO₂ absorption for post-combustion CO₂ capture. Finally, she answered all the questions from the virtual audience and thanked everyone.

The second talk of Session I (Day-IV) began at 10.20 AM, and the resource person was **Dr. Indrajit Paul (Postdoc, University of California, Los Angeles, USA)**. **Dr. Rahul Pal** welcomed the virtual audience and expressed gratitude to **Dr.**

Indrajit Paul for being the invited speaker for the **virtual international conference CCVG-2025**. Dr. Rahul Pal also provided the audience with an overview of Dr. Indrajit Paul's academic background through virtual presentations.

Dr. Indrajit Paul expressed his gratitude to the audience, the organizers, the Principal, the Vice Principal, and the Management of MITS Madanapalle for the invitation from MITS, Madanapalle. He delivered a talk on "**Triplet Sensitized Quantum Amplification in Crystalline Solids**". The topic of his discussion is described below. The phenomenon of triplet sensitized quantum chain amplification in crystalline solids represents a significant advancement in the field of photochemistry and materials science. This process involves the generation and propagation of triplet excitons within a crystalline lattice, leading to a cascade of energy transfer events that amplify the initial photonic input. To that end, we have used the adiabatic valence-bond isomerization of a Dewar benzene (DB) to its corresponding Hückel benzene isomer in mixed crystals grown with a tailor-made sensitizer to establish that a triplet exciton carrier leads to quantum chain reactions where every photon results in up to 517 product molecules ($\Phi \approx 517$), with as little as 0.1% of the triplet sensitizer. By contrast, isomorphous crystals of the **DB** diacid lacking a triplet sensitizer showed a less impressive quantum yield of ca. $\Phi \approx 22$. Mixed crystals designed for this study are based on the use of isomorphous ionic auxiliaries both as crystal engineering handles and as triplet sensitizers. By leveraging the inherent structural order and long-range interactions present in crystalline solids, this mechanism enables efficient energy harvesting and conversion, with potential applications in photovoltaics, light-emitting diodes, and quantum information processing.

The first lecture of Session II (Day-IV) began at 10.45 AM, and the resource person was **Dr. Aditi Agarwal (Principal Consultant, Infosys)**. **Dr. Balaji Mohan (Assistant Professor, MITS, Madanapalle)** chaired the last session of **CCVG-2025**. He welcomed the virtual audience and expressed gratitude to **Dr. Aditi Agarwal** for being the invited speaker for the **virtual international conference CCVG-2025**. Dr. Balaji Mohan also provided the audience with an overview of Dr. Aditi Agarwal's academic background. Dr. Aditi Agarwal expressed her gratitude to the audience, the organizers, the Principal, the Vice Principal, and the Management of MITS Madanapalle for inviting her to the conference. She delivered a talk on "**Digital Transformation in Agrochemical R&D**". The topic of her discussion is described below.

The agrochemical industry is facing significant challenges due to the growing global population and increasing food demand, limited arable land, resource depletion, and crop losses caused by pests, diseases, and adverse weather conditions. Agrochemicals, such as fertilizers and crop protection products, play a critical role in enhancing yields, improving crop health, and ensuring food security. However, due to lengthy development cycles, stringent regulatory requirements, and environmental concerns, there is a need for more sustainable and efficient solutions. Accelerated research and development (R&D) efforts, integrated with digital innovations, are transforming the agrochemical industry. Techniques like data management, predictive analytics, computational chemistry, and AI-driven modeling are streamlining the discovery and development of crop protection products, reducing time-to-market and R&D costs. The application of IT solutions enables the development of safer, more effective, and environmentally sustainable agrochemical products, supporting global agricultural productivity and sustainability.

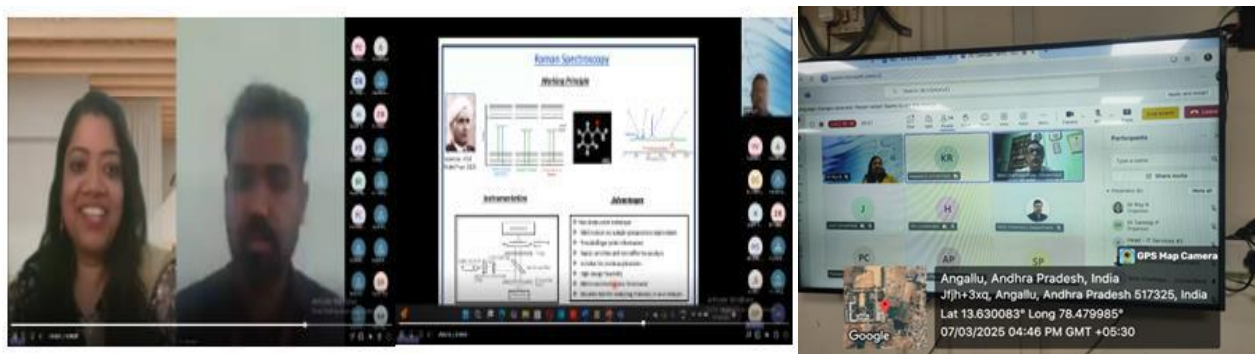


The second lecture of Session II (Day-IV) began at 11.20 AM, and the resource person was **Dr. Prantik Maiti (Group Leader, TCG Lifesciences)**. **Dr. Balaji Mohan** welcomed the virtual audience and expressed gratitude to **Dr. Prantik Maiti** for being the invited speaker for the **virtual international conference CCVG-2025**. Dr. Balaji Mohan also provided the audience with an overview of Dr. Prantik Maiti's academic background. Dr. Prantik Maiti expressed his gratitude to the audience, the organizers, the Principal, the Vice Principal, and the Management of MITS Madanapalle for inviting him to the conference. He delivered a talk on "**Detection techniques of Nitrosamines in various drugs**". The topic of his discussion is described below.

Nitroso impurities, particularly nitrosamines, have been recognized and isolated for several decades. These compounds are present in various everyday items, including food, cosmetics, and pharmaceuticals, at varying levels. Nitrosamines are classified as genotoxic impurities (GTIs), posing significant health risks due to their potential to cause genetic mutations and cancer. Recent advancements in analytical techniques have enabled scientists to detect and quantify these impurities with greater precision. In his lecture, Dr. Prantik Maiti explored several case studies highlighting the detection of nitrosamines in various drugs, the impact of these findings on public health, and the subsequent regulatory actions taken. Additionally, he described the methodologies employed to measure nitrosamine levels in active pharmaceutical ingredients (APIs), including advanced techniques such as liquid chromatography-mass spectrometry (LC-MS) and gas chromatography-mass spectrometry (GC-MS). These methods offer high sensitivity and specificity, enabling the accurate quantification of trace levels of nitrosamines.

The third lecture of Session II (Day-IV) began at 12.05 PM, and **Dr. Sanoop P. (Assistant Professor, Department of Chemistry, MITS, Madanapalle)** was the invited speaker for this session. **Dr. Balaji Mohan** welcomed **Dr. Sanoop P.** at the conference with a brief description of his academic background. Dr. Sanoop P. expressed his sincere acknowledgement

to the audience, the organizers, the Principal, the Vice Principal, and the Management of MITS Madanapalle for giving him a platform to showcase his work. The title of his talk was “*Developing Raman and Surface Enhanced Raman Spectroscopic Techniques for Food and Disease Diagnosis*”. The theme of his lecture is summarized below.



The fourth and last lecture of Session II (Day-IV) began at 12.35 PM, and **Dr. Rashmi Roy (Assistant Professor, Department of Chemistry, MITS, Madanapalle)**, who is also the convener of this conference, was the invited speaker for this session. **Dr. Balaji Mohan** delivered a welcome address to **Dr. Rashmi Roy** at the conference with a short description of her academic achievements. Dr. Rashmi Roy expressed her sincere thanks to the virtual gathering, the organizers, the Principal, the Vice Principal, and the Management of MITS Madanapalle for giving her a chance to demonstrate her work. The title of her talk was “*Strategic Synthesis of Neoglycolipids and Iminosugars*”. The subject matter of her lecture is summarized below. Glycolipids are involved in protein-lipid interactions (with glycan binding proteins) in cell surface and therefore are responsible for various normal and pathophysiological processes in our body. These interactions are responsible for crucial cellular functions. Glycosphingolipids of most Glycosyl Binding Proteins have not yet been identified. The discovery and characterization of biologically relevant GBP-GSL interactions need pure GSLs. Understanding the mechanism of these processes may lead to the development of new anti-infective, anti-cancer, and anti-inflammatory strategies. In 2020, 5 of the top 10 selling drugs were glycosylated drugs and had a combined revenue of \$58 billion USD. The global market for glycomics drugs is supposed to reach \$257 billion USD by 2028. The present work will outline a strategic synthetic approach to obtain novel Neoglycolipids started from the intermediate oligosaccharides available in 1 mg scale. The main objective is to investigate the use of Neoglycolipids (NGLs) as surrogates for GSLs for catch-and-release electrospray ionization mass spectrometry (CaR-ESI-MS)-based screening, inserted in the nanodiscs, for the discovery of new GSL ligands.

The second part of the talk includes synthesis of iminosugars from D-mannitol. Iminosugars are widely used as antidiabetic drugs like Miglustat, Miglitol etc. Therefore, there is always a scope for the synthesis of novel iminosugars and to check their biological activity against the glycosidase enzymes.

The poster session on Day IV began at 3.15 PM. In the poster session, 6 contestants displayed their posters. Each poster presenter gave a presentation of their poster for approximately 8 minutes, and then the judges took questions for 2 minutes to determine which posters were the best based on the novelty of the research work, presentation style, and question-answer session. Around 4.00 PM, the poster presentation was finished.

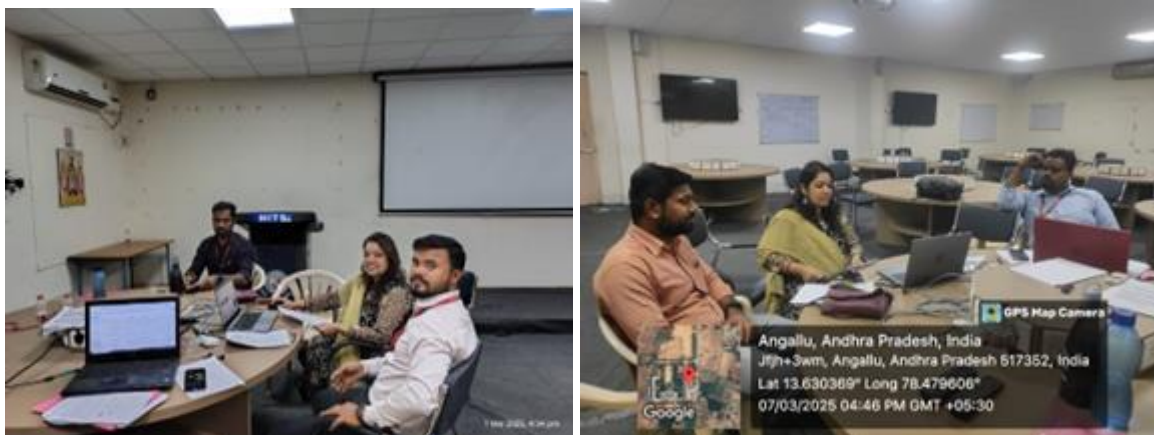
At 4.40 PM, we began the farewell celebration. The HOD, **Dr. Renjith Bhaskaran** gave a few conference-related announcements. Our beloved principal, **Dr. C. Yuvaraj** from the department of mechanical engineering, MITS, was invited by **Dr. Rashmi Roy** to say a few words and declare the ‘**RSC-IPS Young Scientist 2025 Award**’ winners of the virtual poster presentation sessions.



In his brief remarks, the principal expressed his gratitude to the ‘*Indian Photobiology Society*’ for the collaboration, all the faculty members of the department of chemistry, convener Dr. Rashmi Roy, HOD Dr. Renjith Bhaskaran, participants, and invited speakers. Among the 21 posters displayed in the poster section throughout India and internationally, he declared the best poster winners.

Next, the convener, Dr. Rashmi Roy welcomed the vice president of the ‘*Indian Photobiology Society*,’ **Professor Nitin Chattopadhyay (Jadavpur University)**, to address the virtual gathering in the valedictory session. Professor Chattopadhyay is a renowned researcher in the field of photochemistry. Dr. Rashmi Roy gave a brief introduction of Professor Chattopadhyay. Professor Nitin Chattopadhyay gave a vote of thanks to the HOD chemistry department, Principal (MITS),

and management (MITS) for the collaboration. He thanked all the invited speakers, poster presenters, and the participants for actively participating in the conference and for their contribution.



Lastly, our convener, Dr. **Rashmi Roy**, gave a brief vote of thanks to the esteemed invited speakers, delegates, dignitaries, **Indian Photobiology Society, Royal Society of Chemistry, Wiley-VCH, Cambridge Scholar Publishing**, Correspondent MITS (Dr. N. Vijay Bhaskar Choudhury), Executive director MITS (Mrs. Keerthi Nadella), Principal MITS (Dr. C. Yuvraj), Vice principal academics MITS (Dr. P. Ramanathan), Vice principal administration MITS (Dr. C. Kamal Basha), all the supporting staffs of MITS, IT cell, PRO, MITS Radio Station, all the attendees and all the faculty members of Dept. of Chemistry. Finally, Convener Dr. Rashmi Roy formally concluded the conference at 5:30 PM.