Brief Report on the International Symposium on

Chemistry for a Sustainable Future: Bridging Science and Society

held on **13-14 December 2024**

Organized by the Department of Chemistry,

Sri Sathya Sai Institute of Higher Learning

The symposium began with vedam invocation. This was followed by the ceremonial lighting of the lamp by the Vice-Chancellor and the distinguished guests.

Prof. Rajni Bhandari, Head, Department of Chemistry welcomed the guests and the participants to the two-day International Symposium. She provided a thoughtful introduction to the symposium's theme, emphasizing the transformative role that chemistry can play in addressing global sustainability challenges.

A brief summary of the talks delivered as part of the International Symposium is given below.

Prof. B. Raghavendra Prasad,
Vice-chancellor, Sri Sathya Sai Institute of Higher Learning, Prasanthi Nilayam

Bhagawan Baba, our revered founder Chancellor, was a fervent advocate for nature and sustainable living. He championed sustainable development with a focus on energy and health. This symposium serves as a pivotal platform to explore how chemistry can address critical global sustainability challenges. Recent industry interactions highlighted the pressing need for clean energy, emphasizing that 'green' energy sources can still have environmental impacts. Decarbonization is a paramount challenge. In our Institute, we actively strive to reduce our carbon footprint through our dedicated 'Green Cell.'

Chemistry underpins all 17 UN Sustainable Development Goals (SDGs) and the 5 C's of sustainability: Cleanliness, Community, Culture, Care, and Corporate Governance. This symposium should not be merely an academic exercise. We encourage experts and faculty to collaborate and develop a concise symposium outcome statement. We aim to inspire young minds through collaborative discussions and foster impactful actions towards a better future.

The Sri Sathya Sai Central Trust (SSSCT) initiated "Go Green" projects decades ago, reflecting our founder's deep respect for nature, mirroring the reverence for nature found in ancient scriptures. The SSSCT's efforts have significantly increased the green cover in this otherwise arid region of Rayalaseema. We have embarked on several large-scale solar projects. We strive to be an exemplary model in sustainable practices. We anticipate that this symposium will provide a clear roadmap for our Institution to advance its "Go Green" and "Go Clean" initiatives.

"Electrosynthesis: An Emerging Green and Powerful Strategy in Organic Synthesis"

Prof. Goutam Brahmachari
Laboratory of Natural Products & Organic Synthesis, Department of Chemistry,
Visva-Bharati University, Santiniketan, West Bengal

Pioneering advances in green chemistry and engineering are directed towards a sustainable future that is highly demanding for our survival. The ultimate motto of the chemical fraternity is also thus extensively linked with this goal. Synthetic organic chemists are primarily concerned with chemical compounds/materials and their synthetic processes on which the material basis of a sustainable society is largely dependent. Hence, designing for chemical products and processes should follow principles that make them conducive to life.

As part of applying green tools, organic electrosynthesis has become influential in modern synthetic chemistry and finds practical applications in academia and industry due to low energy consumption, mildness, and environmental friendliness. Organic electrochemistry has led to a boom in new synthetic methodologies and their mechanistic understandings. Electrosynthesis has already led to several unprecedented methods. Much of the promise of such a technique hinge on their ability to achieve unique bond constructions that are not feasible using established protocols. Thus, synthetic chemists have been motivated to exploit electrosynthesis to develop efficient strategies for potential organic small molecules. Still, this spectacular field of research is growing in the scenario of global chemical research. As part of the institute's ongoing research endeavours, we have also been deeply involved in green chemistry research during the last few years, focusing on designing and developing new approaches for biologically promising organic small molecules, including the exploration of electrochemical strategies in implementing a handful of organic transformations of interest.

As part of the ongoing research endeavours, we have also been deeply involved in green chemistry research during the last few years, focusing on designing and developing new approaches for biologically promising organic small molecules, including the exploration of electrochemical strategies in implementing organic transformations of interest. In recent years, our group has already published a handful of such research articles in the frontline international journals of repute. The developed electrochemical strategies yielded several series of biorelevant organic molecules, particularly heterocyclic compounds, based on C-H functionalization.

"Chemical Concepts and their Role in Designing Nanomaterials for Energy and Environmental Applications"

Prof. K.R.S. Chandrakumar
Scientist 'G', Bhabha Atomic Research Centre,
Department of Atomic Energy Homi Bhabha National Institute, Mumbai, Maharashtra

Computational chemistry plays a crucial role in the design of nanomaterials for sustainable technologies. It provides quantitative estimates of key parameters like heats of formation, reaction enthalpies, entropies, and reaction rates, which are crucial for understanding chemical reactions and complex systems such as enzyme catalysis and protein dynamics.

Quantum mechanical methods, including Hartree-Fock theory, density functional theory (DFT), and the Born-Oppenheimer approximation, are employed to model molecular behaviour. The Hamiltonian operator is central to describing system energy, particularly in electron synthesis.

The Hard and Soft Acids and Bases (HSAB) principle aids in predicting molecular interactions and guides the design of materials for energy storage and catalysis applications. Key concepts such as hydrogen bonding, proton affinity, and aromaticity are essential for understanding molecular interactions. The curved structures of materials like fullerenes and carbon nanotubes (CNTs) contribute to their unique reactivity and enhanced catalytic capabilities in processes such as ammonia formation. Hydrogen is a promising alternative energy source, although challenges in thermodynamics, kinetics, and storage remain.

As computational chemistry continues to advance, it will play an increasingly vital role in developing innovative nanomaterials and processes that contribute to sustainable energy and environmental applications.

"Development of Efficient Heterogeneous Catalysts for Transfer Hydrogenation, Carbon Dioxide Conversion and Plastic Upcycling Reactions"

Prof. Venkata Krishnan
School of Chemical Sciences, IIT Mandi, Himachal Pradesh

Energy crisis and environmental deterioration has emerged as major problems around the world in recent times, mainly due to combustion of fossil fuels and their depletion. The utilization of light and thermal energy to produce chemical fuels is an attractive and major strategy to address the global energy crisis and other environmental issues. Prof. Venkata Krishnan's research group has developed several two-dimensional materials based on semiconductors, plasmonic materials, perovskite structures and upconversion nanoparticles for energy generation and environmental remediation applications. In addition to photocatalytic hydrogen generation, nitrogen fixation and pollutants degradation, the research group has also utilized these materials for Green organic transformations like transfer hydrogenation, carbon dioxide conversion and plastic upcycling reactions either by decoration, functionalization or doping with a heteroatom. The highlights of the ongoing research work of the group were presented.

A key highlight of the team's success is valorizing saccharides into platform chemicals like 5-hydroxymethylfurfural (5-HMF) using eco-friendly solvents. The research group has also achieved catalytic transfer hydrogenation processes using bio-derived materials, marking a significant advancement in green chemistry. Another standout moment was the use of non-noble catalysts to recycle PET waste into high-value compounds like dimethyl terephthalate (DMT), offering a sustainable approach to plastic waste management. A broader vision of sustainability was presented, aligning the research teams research with the principles of green chemistry and supporting circular economy practices. By leveraging renewable resources and waste materials, the work provides actionable solutions to global challenges like resource efficiency, waste management, and climate change mitigation.

"Aligning Clean Air and Climate Action: Selected Insights from a Decade of Atmospheric Chemistry Research Over South Asia to Foster Transdisciplinary Research"

Prof. Vinayak Sinha
Department of Earth and Environmental Sciences, IISER Mohali, Punjab

The talk majorly focussed on the control of climate and air quality by atmospheric chemical composition, global and Indian outlook on climate and air quality metrics, nano/molecular-level fingerprinting approaches in atmospheric chemistry, and scientific solutions to current environmental challenges. The complicated and interlinked interaction between atmospheric chemistry, climate change, and air quality was highlighted. These issues call for innovative solutions coupled with collaborative research.

VOCs and their oxidized derivatives from human-driven chemical emissions are major contributors to global warming and air pollution. The formation of SOAs and ozone increase climate forcing and health risks. The concept of wet-bulb temperature was discussed to underline the increasing dangers of extreme heat and humidity, especially for outdoor workers.

The presentation demonstrated high-tech tools and techniques that include molecular-level fingerprinting and sophisticated instrumentation for determining atmospheric gases and aerosols. These advancements allow for the very accurate characterization of emission sources and atmospheric processes, providing critical information on their interactions with climate and air quality. Examples of such techniques include the use of UV spectroscopy in measuring ozone, NO_2, SO_2, and PM 2.5, which are considered integral to data-driven policymaking.

Case studies such as the agricultural residue burning in Punjab and Delhi's vehicle policy were presented to illustrate the real-world impact of atmospheric chemistry research. The examples underpin the urgent need for targeted interventions to mitigate emissions from certain sources.

Action-oriented solutions, such as shifting to cleaner sources of energy, waste management improvement, and the use of modern technologies for pollutant removal were presented. Reduction of agricultural burning emissions and cleaner transportation was emphasized. These are necessary steps for sustainable air quality improvement and climate change mitigation.

"Materials and Processes for Energy Storage Applications"

Dr. B. Venkata Sarada.
Scientist 'F', Centre for Solar Energy Materials, International Advanced Research Centre for Powder Metallurgy & New Materials, Hyderabad, Telangana

The presentation highlighted the pivotal role of materials and processes in advancing energy storage solutions for a sustainable future. Her research, centered on nanomaterials, bridges the gap between scientific discovery and practical applications, particularly in electric vehicles (EVs) and stationary storage for renewable energy. The importance of efficient energy storage systems, like batteries and supercapacitors, which are essential for harnessing renewable energy and ensuring a steady power supply were discussed. Various types of batteries, including Na-ion, Li-ion, and Li-S, were compared noting their respective advantages and challenges. Nanomaterials are crucial in enhancing the performance of these devices. The safety concerns around battery fires, especially in electric two-wheelers, were also addressed and safer materials like lithium iron phosphate were recommended.

Manufacturing techniques, such as ball milling, to improve battery efficiency and reduce production costs was presented. The innovative research in supercapacitors at ARCI and ARO, underscoring the importance of advanced materials and processes in achieving efficient, reliable energy storage systems for a sustainable energy future was highlighted.

"Surfaces Solutions as Enablers for Sustainable Manufacturing"

Dr. Vishal Khetan
Global Innovation Manager Coatings, Oerlikon Surface Solutions AG, Liechtenstein.

Along with the new generation manufacturing, climate change and energy challenges, surface engineering will phase in a new era of research and innovation. It is desired that the new technologies such as physical/chemical vapour deposition (PVD, CVD) of surfaces used in multiple manufacturing industries such as automotive, medical, packaging and aerospace can be addressed and introduced to a broader industry perspective.

Tribology and Surface Engineering, as enabling technologies, have been continuously advancing global manufacturing sectors in terms of fuel economy (reduced friction and wear), improved productivities and product reliability, functionalisation of machine components, providing alternative manufacturing processes due to environment legislations, and electrification of vehicles, etc.

The talk focused on fundamentals and new innovations in Surface Engineering for conventional manufacturing systems and applications of Tribological Systems in industry (medical, oil & gas, aerospace, automotive, engineering, electrical vehicles, etc) to drive sustainability in manufacturing industry. Specifically, BALINIT® MAYURA, a product developed and launched by Oerlikon Surface solutions AG was used as an example to illustrate how to drive sustainability within the organisation. Further, some case studies to illustrate sustainable practices in industry were presented.

"Swami, Sun & Sustainability: Materials for Solar-Thermal Conversion"

Prof. Chandramouli Subramaniam
Department of Chemistry, IIT Bombay, Mumbai, Maharashtra

The urgent need for sustainable innovation to address global warming caused by rising CO_2 emissions since the industrial revolution was highlighted. The focus was on solar energy as a clean and abundant solution to mitigate CO_2 emissions and convert "red heat" into "green heat." A breakthrough in solar-thermal conversion technology, designing black-body absorbers made from vertically aligned carbon nanotubes with bamboo-like structures was presented. This design can capture over 98% of the solar spectrum, including infrared. Integrated into silica-coated materials, it led to the creation of "Aditya," a solar water heater prototype. This device offers practical benefits, including contactless bactericidal water purification, reduced carbon footprints, and the prevention of biofouling—key to global efforts for clean water and energy. The presentation also emphasized the ethical responsibility of using technology to improve humanity's well-being. His work connects advanced materials and renewable energy to crucial issues like health, climate resilience, and sustainable development, inspiring a vision of a future where science and society thrive together.

"The Frontiers of AI Research"

Dr. Sampath Koppole
Products and Solutions Lead, Healthcare and Life Sciences, Google, Switzerland.

AI has to be built responsibly and to benefit humanity. AI is a very useful, focused tool that makes work processes more productive. AI as a tool should serve the focused purpose and must make a positive impact. We need to be very careful about its usage and the capacity. AI helps in various capacities and enhances the productivity. It has impact on every aspect of our life and is used everywhere be it email writing or workspace. It is a very useful tool for scaling up our work. The main goal is to see how it can serve the humanity better and help in a better way.

It has capacity to do any work in a better and time efficient manner. The Nobel prize is also given in the various disciplines by combination of fundamental research with the AI. Be it image, text, sound, video etc. it has the multimodality capacity.

GNoME-Graph Networks for Material Exploration is an important AI tool for generating new materials. AI generated materials with better electromechanical properties for electronics and energy storage are available in the GNoME database and are publicly available. The machine was further used to generate recipes for synthesis of the materials. A high success rate of 71% was achieved for the synthesis of computationally predicted materials.

GraphCast is an AI model for weather prediction. The current systems for weather prediction are extremely computationally intensive. For every 25 degrees, i.e. 28 by 28 kms, weather patterns are predicted based on the current weather inputs taking five different weather variables.

AlphaFold creates a three-dimensional view of the protein from a given sequence of amino acids. This got the Nobel prize recently. Human biology runs with proteins. Knowledge of the structure is central to understanding its function and properties. Small molecules can then be created to modulate the functioning of proteins. Over 200 million protein structures are available in the database today. Knowledge of protein structure has multitude of applications such as customized pesticide creation, plastic management, etc. **AlphaFold 3** is a tool for modeling the genome sequence. AlphaFold was combined with genomics for possible disease prediction.

Overall, the field of AI provides a very good opportunity to explore and increase the understanding of the chemistry of the different materials and molecules.

A presentation showcasing the research activities and advancements of the department was made by faculty representative on Day 1. This session offered a glimpse into the ongoing efforts and achievements of our research groups.

The afternoon session on Day 2, was a vibrant display of creativity and talent:

- Student clubs presented live demonstrations, showcasing practical applications of sustainable practices in chemistry. Their enthusiasm and ingenuity were a testament to the promise of the next generation of scientists.

- This was followed by a poster presentation by undergraduate and postgraduate students, covering a wide range of topics related to sustainability through chemistry. These presentations offered an opportunity to appreciate the diversity of ideas and the dedication of our budding researchers.
- Senior doctoral research scholars delivered concise and impactful presentations on their ongoing research within the department

The International Symposium concluded with Mangala Aarthi to Bhagawan Sri Sathya Sai Baba.

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