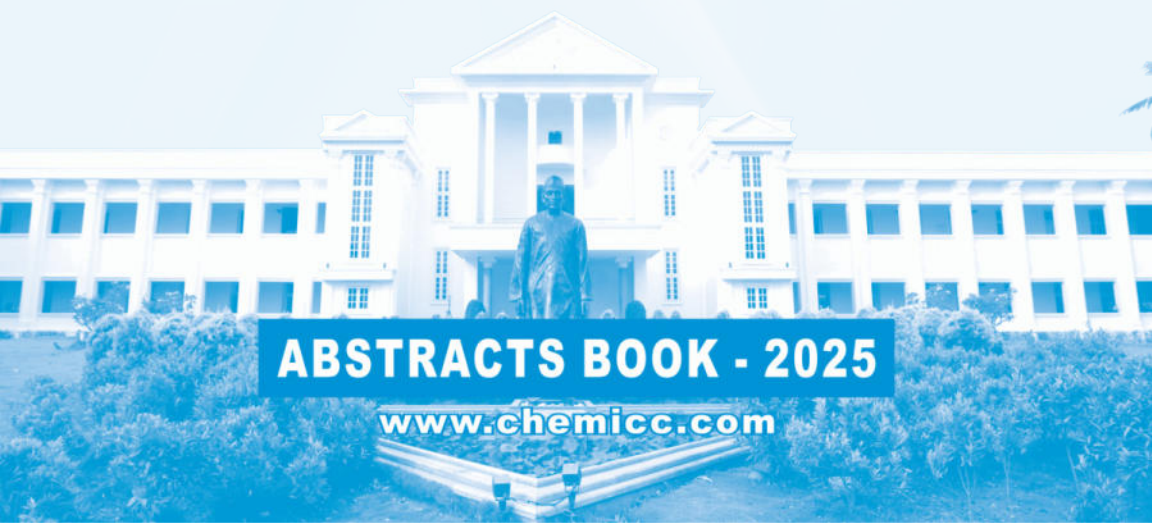




**XXXXIV**  
**ANNUAL CONFERENCE**  
**INDIAN**  
**COUNCIL OF CHEMISTS**  
**22<sup>nd</sup> - 24<sup>th</sup> DECEMBER, 2025**



**School of Advanced Sciences**  
**KLE Technological University BVBCET Campus**  
**Vidyanagar, Hubballi-580031, Karnataka**



**ABSTRACTS BOOK - 2025**

**[www.chemicc.com](http://www.chemicc.com)**

## CONFERENCE COMMITTEE

**Dr. Greesh Saxena**  
Patron, ICC, Ex. V.C.  
78, North Vijay Nagar, Agra-282004

**Prof. Ranjeet Kr. Verma**  
President, ICC  
Founder V.C. Munger Uni.,  
69, A.P. Colony, Gaya-823001

**Prof. Rajesh Dhakarey**  
Secretary, ICC  
Ex. Vice Chancellor  
Maharaja Surajmal Brij University  
Bharatpur-321201 (Rajasthan)

**Prof. M.K. Rawat**  
Treasurer, ICC  
Principal, Meerut College,  
Meerut-250 001 (U.P.)

**Prof. Ajay Taneja**  
Zonal Secretary, ICC  
Vice-Chancellor  
Khwaja Moinuddin Chishti  
Language University, Lucknow

**Dr. S.C. Goyal**  
Joint Secretary, ICC  
Former Head, Department of Chemistry  
Agra College, Agra-282002

**Prof. Vinod Kumar**  
Joint Secretary, ICC  
Department of Chemistry,  
Agra College, Agra-282 002

## SECTIONAL PRESIDENTS

### ANALYTICAL AND ENVIRONMENTAL CHEMISTRY SECTION

**Prof. Annamalai Senthil Kumar**

Nano and Bio-electrochemistry Research Laboratory, Department of Chemistry,  
School of Advanced Sciences and CO<sub>2</sub> Research and Green Technology Centre,  
Vellore Institute of Technology University, Vellore-632 014, Tamil Nadu

### INORGANIC CHEMISTRY SECTION

**Prof. Vinod Kumar Sharma**

Department of Chemistry, University of Lucknow, Lucknow-226007

### ORGANIC CHEMISTRY SECTION

**Prof. Arun M. Isloor**

Department of Chemistry  
National Institute of Technology, Suratkal, Karnataka

### PHYSICAL CHEMISTRY SECTION

**Prof. Ramesh L. Gardas**

Department of Chemistry, IIT-Madras, Chennai-600036 (T.N.)

### SYMPOSIUM ON "RECENT ADVANCES IN POLYMER SCIENCE AND TECHNOLOGIES - EMERGING MULTIFUNCTIONAL POLYMERIC MATERIALS

**Prof Tejraj M. Aminabhavi**

Director of Research, Center for Energy & Environment  
School of Advanced Sciences, KLE Technological University,  
BVB-CET Campus, Vidyanagar, Hubballi -580031, Karnataka

# INDIAN COUNCIL OF CHEMISTS



[www.chemicc.com](http://www.chemicc.com)

**XXXXIV  
ANNUAL NATIONAL CONFERENCE  
2025**

## **ABSTRACTS BOOK**



School of Advanced Sciences  
KLE Technological University  
BVBCET Campus, Vidyanagar  
Hubballi-580031, Karnataka

**22<sup>nd</sup> - 24<sup>th</sup> DECEMBER, 2025**

*Editor : Prof. Rajesh Dhakarey*

## **Welcome**

**Dear Fellow Researchers & Scientists**

*On behalf of the Indian Council of Chemists, it is my pleasure and honour to welcome you all to the XXXXIV Annual Conference of ICC from 22<sup>nd</sup> - 24<sup>th</sup> December, 2025 at School of Advanced Sciences, KLE Technological University, BVBCET Campus, Vidyanagar, Hubballi-580031, Karnataka*

*The leading researchers and key opinion leaders in Chemistry have been invited to facilitate sessions and deliver lectures at XXXXIV Annual National Conference of ICC.*

*There will be vast range of learning opportunities at invited talks, oral, poster presentations and symposium session. Participants can also look forward to expanding their network at various networking events such as conference lunch, dinner and cultural programme. Apart from the scientific programme, there are many tourist attractions in and around Hubballi (Karnataka). You can enjoy there too.*

*Thank you for your participation.*

**Prof. Rajesh Dhakarey**  
Secretary, ICC

## **PROVISIONAL PROGRAMME**

### **Monday, December 22nd, 2025**

08.00 to 09.30 am	Registration
09.30 to 01:00 pm	Inauguration, keynote address
01:00 to 02:00 pm	Lunch
02:00 to 02:30 pm	Sectional Presidents address in respective sections
02:30 to 05:30 pm	Invited lectures and paper presentations
05:30 to 07:30 pm	Poster presentations and Executive Meeting
07:30 to 08.45 pm	Cultural programme
08:45 pm onwards	Dinner

### **Tuesday, December 23rd, 2025**

09:00 to 1:00 pm	Symposium on "Recent Advances in Polymer Science and Technologies - Emerging Multifunctional Polymeric Materials" (common to all delegates)
01.00 to 02.00 pm	Lunch
02:00 to 06:00 pm	Invited lectures and paper presentations
06:00 to 07:30 pm	Poster presentations
07:30 to 08:30 pm	ICC General Body Meeting (To be attended by fellows only)
08:30 pm onwards	Dinner

### **Wednesday, December 24th, 2025**

09:00 to 01:00 pm	Invited lectures and paper presentations
01:00 to 02:00 pm	Lunch
02:00 to 04:00 pm	Invited lectures and paper presentations
04.00 to 06.00 pm	Valedictory Function

The detailed programme of each day and each section shall be circulated in the Conference.

## ADVISORY COMMITTEE

### Chief Patrons

**Dr. Prabhakar Kore**  
Chancellor

**Prof. Ashok Shettar**  
Pro-Chancellor

### Patron

**Prof. Prakash G. Tewari**  
Vice-Chancellor

### Conference Chair

**Prof. Tejraj M. Aminabhavi**  
Director of Research

### Conference Co-Chairs

**Prof. B. L. Desai**  
Dean Executive

**Prof. Basavaraj B. Kotturshettar**  
Dean Academics

**Prof. Uma Mudenagudi**  
Dean R & D

**Prof. Basavaraj S. Anami**  
Registrar

**Prof. N. H. Ayachit**  
Dean Science & Technology

**Prof. Sanjay Kotabagi**  
Dean Student Welfare

### Convenor

**Prof. Nagaraj P. Shetti**  
School of Advanced Sciences  
KLE Technological University, Vidyanagar, Hubballi 580031, Karnataka  
Mob.: 9611979743, E-mail: npshetti@kletech.ac.in

### Organizing Secretary

**Prof. Nagaraj R. Banapurmath**  
Center for Material Science  
KLE Technological University, Vidyanagar, Hubballi 580031, Karnataka  
Mob.: 9880726748, E-mail: nr\_banapurmath@kletech.ac.in

### Joint Organizing Secretaries

**Dr. Shweta J. Malode**  
Center for Energy & Environment

**Dr. Sandeep R. Kurundawade**  
Dept. of Chemistry

**Dr. Deepak A. Yaraguppi**  
Dept. of Biotechnology

## Instructions for the Preparation of Poster Presentation

The poster should be displayed as per the poster board number given in the abstract book. Posters will be displayed during the Poster Sessions and must be mounted from the start of sessions and removed upon conclusion of sessions on the scheduled day. Authors are requested to stand next to their poster boards during the Poster Sessions.

- You should be printing and bringing your poster to the conference.
- The dimensions of poster **should NOT exceed 90 cm wide × 120 cm high.**
- Please prepare your poster to fit the dimensions specified. It is recommended that poster be prepared on one sheet. Alternatively presenters may display their material on several smaller sheets.
- Allocate the top of the poster for the title and authors as stated on the submitted abstract.
- The text, illustrations, etc. should be bold enough to be read from a distance of two meters.
- Double sided tape and technical equipment will be available for the mounting of posters. Staff will also be available to assist you.
- DO NOT write or paint on the poster boards. DO NOT use nails, push pins, screws, or any tools that will puncture the poster boards.
- Please use the board that displays the same number assigned to you.

For any help kindly contact the concerned **Sectional President** or **Prof. Ajay Taneja**, Zonal Secretary-ICC.

## ***Acknowledgements***

*The Indian Council of Chemists is going to held its XXXIV Annual Conference at Hubballi on 22<sup>nd</sup>-24<sup>th</sup> December, 2025 and the abstract book containing the abstracts of papers selected for presentation in the Conference is in your hands. The Council justifiably feels proud of its achievements during the past 44 years of its existence.*

*The Council is grateful to Staff Members and Students of School of Advanced Sciences, KLE Technological University, BVBCET Campus, Vidyanagar, Hubballi-580031, Karnataka for their utmost cooperation in organizing the Conference.*

*The Council on its own behalf and on behalf of the Organizing Committee thanks all those who have helped in preparing and publishing this Abstract Book. The assistance given by Prof. Manoj Rawat, Dr. S.C. Goyal, Prof. Vinod Kumar, Dr. Bhoopendra Singh and Prof. Ajay Taneja is gratefully acknowledged.*

*Some of the abstracts have been edited by Sectional Presidents; due to paucity of funds and pressing limitations on space, a few others have been condensed, and some inadvertent omissions might have occurred for which ICC offers its apologies.*

*We are very much thankful to our Sectional Presidents and Convenor of the Symposium for untiring work in compilation of this abstracts book. I have tried to include all the abstracts received from Sectional Presidents till 4<sup>th</sup> December; however, if any abstract is missing, bear with me it may be included in the soft copy after the Conference.*

***Prof. Rakesh Dhakarey***  
*Editor*



### ***Welcome note from the President***

*Welcoming distinguished scientists, guests and the participants to the XXXIV Annual Conference of the Indian Council of Chemists is extremely delighting to me. This is being hosted by the School of Advanced Studies, KLE Technological University, Hubballi, Karnataka during December 22-24, 2025.*

*The Indian Council of Chemists through its annual conferences, takes the lead every year in holding the nation's biggest and the most prestigious annual chemistry event which is known for its remarkable versatility and visibility across institutions in India. Being the apex national body of Chemistry, ICC has thousands of members and Fellows on its roll spreading all over the country. Its Annual Conference is regarded as the annual epicenter for dissemination of new research ideas in Chemistry generated in the country. It brings together, the researchers, academicians, and industry professionals providing immense opportunities to the young and budding scientists to rub shoulders with the Who's Who in the respective fields. Everyone has chances to get inspired and take up new research ventures and enter into new collaborations.*

*Widening its activities, last year ICC started celebrating annually, the 2<sup>nd</sup> of August-the birthday of Acharya P. C. Ray (August 2, 1861 – June 16, 1944) as the National Chemistry Day. Acharya Ray who is revered as the “Father of Indian Chemistry” was a true inspiring patriotic and motivational chemist with rare entrepreneurships, research and organizational skills. He was also the first Indian scientist whose research paper was published in modern times on the basis or work carried on in India. This year too, the Chemistry Day (NCD-2025) was celebrated like a movement in Universities, Colleges and Schools on August 2, 2025, across the length and breadth of the country. Some other organizations have also started taking up the celebrations. ICC is making efforts for declaration of this day as the “National Chemistry Day”. Best performing institutions are being recognized by ICC this year too. New activities aiming at patronizing quality research in Chemistry and popularizing Chemical Sciences are being planned.*

*Like previous years, a Symposium is also being organized during this conference. The title is, “Recent advances in polymer science and technologies - emerging multifunctional polymeric materials”. This will be besides the presentations in the main Sections chaired by leaders in the respective fields. We are sure, you would enjoy the deliberations and events and their spirits. I wish the conference a grand success.*

***Ranjit K Verma***  
***ICC***

## **CONTENTS**

Symposium	01-07
Analytical and Environmental Chemistry Section	08-76
Inorganic Chemistry Section	77-131
Organic Chemistry Section	132-187
Physical Chemistry Section	188-246

## **ABBREVIATIONS**

AEIL	- Analytical Invited Lecture
AEO	- Analytical Oral
AEP	- Analytical Poster
IIL	- Inorganic Invited Lecture
IO	- Inorganic Oral
IP	- Inorganic Poster
OIL	- Organic Invited Lecture
OO	- Organic Oral
OP	- Organic Poster
PIL	- Physical Invited Lecture
PO	- Physical Oral
PP	- Physical Poster
CYSA	- Contestant for Young Scientist Award
SYM-SP	- Symposium

## AWARDEE 2025



**Prof. Tejraj M. Aminabhavi**  
Life Time Achievement Awardee



**Prof. Sheshanath Vishwanath Bhosale**  
Prof. W.U. Malik Memorial Awardee



**Prof. Yogesh Chandra Sharma**  
Dr. S.P. Hiremath Memorial Awardee



**Dr. Nilanjan Dey**  
Dr. Arvind Kumar Memorial Awardee



**Prof. Saiqa Ikram**  
Prof. Kaza Somsekhara Rao Awardee



**Prof. Rajesh K. Vatsa**  
Prof. S.T. Nandibewoor Awardee



**Dr. Arvind Singh Negi**  
Dr. S.M.L. Gupta Memorial Awardee



**Prof. Pragnesh N. Dave**  
Dr. P.N. Sharma Memorial Awardee

## SECTIONAL PRESIDENTS



**Prof. Tejraj M Aminabhavi**

Symposium on  
"Recent Advances in Polymer Science  
and Emerging Multifunctional  
Polymeric Materials"



**Prof. Vinod Kumar Sharma**  
Inorganic Chemistry Section



**Prof. Arun M. Isloor**  
Organic Chemistry Section



**Prof. Ramesh L. Gardas**  
Physical Chemistry Section



**Dr. Annamalai Senthil Kumar**  
Analytical and Environmental  
Chemistry Section

## CONFERENCE COMMITTEE



**Dr. Greesh Saxena**

Patron, ICC, Ex. V.C.  
78, North Vijay Nagar, Agra-282004



**Prof. Ranjeet Kr. Verma**

President, ICC  
Founder V.C. Munger Uni.,  
69, A.P. Colony, Gaya-823001



**Prof. Rajesh Dhakarey**

Secretary, ICC  
Ex. Vice Chancellor  
Maharaja Surajmal Brij University  
Bharatpur-321201 (Rajasthan)



**Prof. M.K. Rawat**

Treasurer, ICC  
Principal, Meerut College,  
Meerut-250 001 (U.P.)



**Prof. Ajay Taneja**

Zonal Secretary, ICC  
Vice-Chancellor  
Khwaja Moinuddin Chishti Language  
University (KMCLU), Lucknow



**Dr. S.C. Goyal**

Joint Secretary, ICC  
Former Head, Department of Chemistry  
Agra College, Agra-282002



**Prof. Vinod Kumar**

Joint Secretary, ICC  
Department of Chemistry,  
Agra College, Agra-282 002

## **Life Time Achievement Awardee Lecture**

### **Polymeric Materials in Health, Energy and Environment**

**Tejraj Aminabhavi**

*Center for Energy and Environment, School of Advanced Sciences  
KLE Technological University, Hubballi 580 031  
E-mail : aminabhavit@kletech.ac.in*

Development of new polymers and materials required in industrial sectors for environmental applications, membrane separations and biomedical areas are being actively pursued over many decades. Among the polymeric materials that deserve to be highlighted as different types of polymers and materials for the benefit of mankind such as adsorption of contaminants (pesticides, potentially toxic metals, and medicines, among others) to provide clean environment for health benefits. Photocatalytic polymers and materials, surface coatings without the degradation of organic compounds in water, polymeric membranes used for filtration of toxic contaminants in water media for the restoration of ecosystems and release of specific compounds, biodegradable plastics for renewable resources and conducting polymers in renewable energy storage and energy production areas as well developing polymers in biomedical fields such as drug delivery systems, targeted therapy, scaffolds in tissue engineering, implantation of medical device artificial organs, prosthesis, ophthalmology, dentistry, bone repair, and many other medical fields are the outcomes of research efforts around the world. Owing to good biocompatibility and easy modification, natural polymers are now a great interest in biomedical applications. Similar efforts are being pursued in developing novel materials required in energy production technologies. Representative examples of these areas are covered briefly.

**To be presented as  
Key Note Address**

## **Prof. W.U.Malik Memorial Awardee Lecture**

### **Development of Nano- and Bio-technological Tools using Supramolecular Chemistry**

**Sheshanath Vishwanath Bhosale**

*UGC-FRP Professor, FRSC, FMASc, MRACI, ARC-Future Fellow & ARC-APD School of Chemical Sciences, Central University Karnataka, Kalaburgi-585367*

*E-mail: bsheshanath@cuk.ac.in; bsheshanath@gmail.com*

In this award lecture, Prof. Bhosale describe supramolecular self-assembly in both basic and applied research, especially the construction of nano- and bio-technological tools for various applications such as removal of environmental toxic pollutants, drug-delivery, cancer treatment, photosynthesis and optoelectronic devices. Also give depth of the use of small organic molecules with their self-assembly to create supramolecular chiral structures from achiral molecules has given a true depth of understanding to the biological world. In particular, will also give depth of in the field of Supramolecular Organic Nanomaterial and has constantly devoted his research in the following areas:

i) Development of nanoparticles for a cancer cure, especially chemistry of yoctowells, ii) use of NDI and porphyrin functionalization organic molecules for artificial photosynthesis and organic solar cell applications and iii) Use of small organic molecules for supramolecular sensing and photocatalysis applications to remove toxic organic pollutant and ions. Furthermore, this lecture also gives depth of Vanadium pentoxide nanoparticle mediated perturbation in cellular redox balance and paradigm of autophagy to apoptosis”, a breakthrough on breast cancer. In their work study they found that vanadium pentoxide nanoparticles could kill almost 59.60% of cancer cells within 48 hours as compared to just 15.04% cells death in normal fibroblast. Results indicate that the vanadium pentoxide nanoparticles selectively induce breast cancer cell death and hence this drug could be used for breast cancer management. This has been the most crucial challenge for the group, as overcoming chemoresistance that has still remained a hurdle in cancer therapy.

**To be presented in  
Organic Chemistry**

**Prof. S.P. Hiremath Awardee Lecture**

**Adsorption Technology for Sustainable  
Water and Wastewater Treatment: Past,  
Current and Future Scenario**

**Yogesh Chandra Sharma**

*Department of Chemistry, Indian Institute of Technology BHU  
Varanasi, Varanasi 221005*

World is facing problem of pollution globally. If you look into nature, it's a self sustained system, a zero waste generation system. Each waste is a potential food of some specie. Industrialization beyond capacity of nature seems to be its majour reason. Be it water, air or soil: all sources are extremely polluted. In case of water, dyes, heavy metals, antibiotics, polyfluorinated alkyls, and other organic and inorganic constituents are reported to be principal pollutants. The article focusses on application of adsorption technology for treatment of polluted waters and wastewaters. Adsorption has been utilised widely from the past to the present time for reclamation of these contaminant. Activated carbon processes have been most common for wastewater reclamation. But later, adsorbents like calcium oxide, charcoal, and silica gel have been utilised for reclamation frequently. For about a decade, waste materials and minerals were frequently reported for the purpose. But, these materials had some issues. They displayed low adsorption capacity, leaching problems, and low reusability. The new materials, namely nanoadsorbents, mesoporous carbons, metal organic frameworks, hydrogel materials, and superadsorbents are being used with their best physicochemical properties, like surface area, loading capacity (1-2500 mg/g), reusability, and equilibrium time optimisation. These adsorbents, mainly nanoadsorbents, mesoporous carbon and MOF materials, are trending to overcome water and air pollution. Since these are easily preparable from biomass feedstocks and metal ligand moieties. The surface of these materials is in the range of 100-7000 m<sup>2</sup>/g, with variation in porosity according to the adsorbate target. Through PXRD, RAMAN, HR-TEM, SEM, BET/BJH, AND UV-vis spectrophotometer study, removal of pollutants like dyes and heavy metals can be assessed. So, the presentation has these issues as a priority to be focused on.

**To be presented in  
Analytical Chemistry Section**



**Dr. Arvind Kumar Memorial Awardee Lecture**

**Designing Pyrimidine-Based Probes for a Sustainable Future: Bridging Food, Agriculture, and Diagnostics through Smart Chemical Sensing**

**Nilanjan Dey**

*Department of Chemistry, BITS-Pilani Hyderabad Campus,  
Shameerpet, Hyderabad-500078, Telangana  
E-mail: nilanjandey.iisc@gmail.com, nilanjan@hyderabad.bits-pilani.ac.in*

Pyrimidine-based charge transfer (CT) scaffolds provide a unified strategy for chemical sensing by integrating hydrogen-bonding interactions with reactivity-driven pathways. These molecular-level interactions not only modulate CT states but also influence aggregation behavior, enabling versatile sensing outcomes. Amphiphilic CT probes exploited hydrogen bonding between water and the pyrimidine-2,4,6-trione motif to detect trace moisture in soils and leaves with limits as low as 0.17 wt% (v/v). Water-induced aggregate disruption produced ~5-fold fluorescence quenching that remained robust to variations in pH, temperature, and ionic strength. Predictive performance was enhanced by machine-learning regression ( $R^2 = 0.9984$ , RMSE = 0.0166), while smartphone-enabled colorimetry and paper strips provided low-cost, field-deployable monitoring. Extending the platform to biomedical diagnostics, the same probes achieved dual-mode uric acid detection through multipoint hydrogen bonding, showing strong linearity ( $R^2 = 0.998$ ) with a detection limit of 0.12  $\mu\text{M}$ , validated in urine, serum, and live cells. Translation into paper-strip assays further established rapid, point-of-care applicability. Complementarily, orthogonal sensing of glutathione (GSH) and hydrazine ( $\text{N}_2\text{H}_4$ ) was achieved via distinct covalent pathways: Michael addition with GSH (~5-fold quenching, LOD 0.87  $\mu\text{M}$ ) and hydrazinolysis/hydrazone formation with  $\text{N}_2\text{H}_4$  (~22-fold quenching, LOD 0.23  $\mu\text{M}$ ). Distinct absorption shifts, lifetimes, and kinetics validated orthogonality, with applications spanning food washings, enzymatic assays, and biological fluids using portable dipsticks.

**To be presented in  
Organic Chemistry Section**

## **Prof. Kaza Somsekhar Rao Awardee Lecture**

### **Biodegradable Materials for Sustainable Products: Innovations for Self-Resilient Societies**

**Saiqa Ikram**

*Department of Chemistry, Jamia Millia Islamia (Central University)  
New Delhi 110025*

*E-mail : sikram@jmi.ac.in*

Biopolymer based materials pose high potential as sustainable alternatives to synthetic polymers. Cellulose–chitosan-based biocomposites, due to biocompatibility, biodegradability, and antimicrobial properties, attract attention for wide application in various industries. The research work in our lab includes modern methods for producing cellulose–chitosan composites aimed at improving their mechanical and chemical properties. Such recent research on the environmental applications of biopolymers has been comprehensively analyzed, thus providing a fresh insight into the future prospects of research in this domain.

Attention is paid to the use of composites in packaging materials, and adsorbents for wastewater treatment where the composites display high sorption, recyclability/durability, and reducing environmental footprint as compostable materials. They also played pivotal part in other environmental applications including anti-desertification, natural bio-sealants for preventing concrete leaks and proton conducting membranes in electrochemical devices. In medicine, wound dressings prepared for drug delivery and tissue engineering, providing controlled release of active substances and resisting microbial infection resulting a faster healing. The hydrogels and nanocomposites as films have functioned effective biosorbents/ Super-absorbents (SAPs) and have been vastly harnessed as Xerogels for hygienic applications.

Enzyme immobilization technology holds significant value in biocatalysis. Enzyme binding modules with specificity, offer a highly promising immobilization method. The chitosan functionalized magnetic nanocomposites present a nano-

biocatalytic system that enables easy retrieval, separation, and recycling of matrix with enhanced shelf life, thereby offering a cost effective and sustainable approach. These functional nanostructures provide an insight into the synthesis, immobilization, and applications aiming to bridge the gap between sustainable utilization and economic viability by incorporating the emerging nanocomposite immobilization approach.

By comprehensive employments of cellulose–chitosan biocomposites, highlighting their synergistic properties, in line with principles of green chemistry and the United Nations' Sustainable Development Goals, our research also addresses important issues as cost-effective production methods and future innovations, and proposes a roadmap for the introduction of these materials as sustainable alternatives to plastic towards Technology Transfers.

**To be presented in  
Inorganic Chemistry Section**

## Prof. S. T. Nandibewoor Awardee Lecture

### Using Lasers as a Tool in Chemistry

**Rajesh Vatsa**

*Former Head, Structural Chemistry Section, Chemistry Division,  
Bhabha Atomic Research Centre, Mumbai 400085*

Lasers have revolutionized science and technology ever since their discovery. There is hardly any field in science and technology that has not advanced or benefitted from the use of lasers. In this lecture, I will present results wherein lasers were used as a tool to probe chemistry, either deeper or in newer ways to get information which was not available. Examples from work done at BARC and elsewhere will be discussed showing use of lasers in getting new information about chemical species or studying reactions.

During his photodissociation studies on  $\text{CF}_2\text{Br}_2$ , transient radical species  $\text{CF}_2\text{Br}$  was conjectured as an intermediate by Prof. Y.T. Lee (1986 Nobel Laureate in Chemistry). However, no experimental evidence of existence of  $\text{CF}_2\text{Br}$  was provided. Using carefully chosen laser excitation and real time UV absorbance measurements, existence of  $\text{CF}_2\text{Br}$  radical was confirmed by us, its absorption cross-sections (220-280 nm) as well as second order dimerization rate constant were measured.

Isotope exchange reactions are very difficult to study using conventional kinetics techniques. However, lasers with their highly sharp monochromatic emission lines, can overcome this difficulty very easily, thus allowing measurement of the concentration of different isotopes. This method was used to measure rates of isotope exchange model reactions such as  $\text{H}+\text{D}_2$ ,  $\text{D}+\text{HD}$  and  $\text{H}+\text{DCl}$ .

Absorption cross-sections at Lyman-alpha (121.567 nm) wavelength are important to model the ultimate fate of molecules in stratosphere wherein they get photoexcited by the intense Lyman alpha radiation present there. Precise values of cross-sections at 121.567 nm are difficult to measure due to the bandwidth of the radiation source. Absorption cross-sections for several atmospherically important molecules ( $\text{H}_2\text{O}$ , CFCs,

CH<sub>4</sub>, etc.) were measured with an unprecedented resolution of 0.0006 nm. The values are widely cited and are listed as reference values on SCIENCE SOFTCON (<http://www.science-softcon.de/spectra>)

Laser induced ionisation is an important source for selectively creating ions of any element. Results will be presented wherein it will be shown that it can also be used to create surprisingly highly charged ions such as Xe<sup>+</sup> to Xe<sup>+10</sup> using unbelievably low energy laser pulses interacting with xenon vander waal's clusters.

**To be presented in  
Physical Chemistry Section**

**Dr. S.M.L. Gupta Memorial Awardee Lecture**

**Plant Based Microtubule Destabilizers  
as Target Specific Cancer  
Chemotherapeutics**

**Arvind Singh Negi**

*Phytochemistry Division, CSIR-Central Institute of Medicinal and  
Aromatic Plants (CSIR-CIMAP), Lucknow-226015, U.P.  
E-mail: arvindcimap@gmail.com*

Cancer is a prime health threat to mankind. The affordability of treatment is a challenge to a common person. It is the second major cause of human deaths, every year about 10 million deaths which is 17% of total human deaths [WHO, Cancer: Keyfacts, 03 Feb 2025]. There are some naturally occurring microtubule destabilizers like podophyllotoxin, colchicine, and combretastatin A4 as structural learning to design new microtubule destabilizers as cancer chemotherapeutics. In our work, we used Fragment Based Drug Discovery approach (FBDD) approach to design new drug candidates by introducing a 3,4,5-trimethoxyphenyl fragment inducing antitubulin effect [Negi et al. 2015]. We incorporated this fragment in our several diverse pharmacophores and achieved potential antitubulin anticancer effect. Further, one such designed anticancer New Chemical Entity (NCE) as microtubule destabilizer is under GLP grade evaluations for IND filing process. The designing, synthesis and biological evaluation will be discussed in detail.

**To be presented in  
Organic Chemistry Section**

**Dr. P. N. Sharma Memorial Awardee Lecture**

**ANN-Assisted Investigation of the  
Thermal Decomposition Behavior of  
Ammonium Perchlorate/LaMn<sub>0.4</sub>Fe<sub>0.6</sub>O<sub>3</sub>**

**Pragnesh N. Dave**

*Department of Chemistry, Sardar Patel University, Vallabh  
Vidyanagar, 388120, Gujarat*

*E-mail: pragneshdave@rediffmail.com*

Enhancing the thermal decomposition of ammonium perchlorate (AP) through the incorporation of metal oxides has been a subject of continuous research. In this study, the thermal decomposition behavior of AP containing 1 wt% of the tri-metal perovskite oxide LaMn<sub>0.4</sub>Fe<sub>0.6</sub>O<sub>3</sub>, synthesized via the citrate sol-gel method, was investigated at four different heating rates ( $\beta = 5, 10, 15, \text{ and } 20 \text{ }^\circ\text{C min}^{-1}$ ). Artificial neural networks (ANNs) were employed to forecast the decomposition profile of the AP/LaMn<sub>0.4</sub>Fe<sub>0.6</sub>O<sub>3</sub> composition. The ANN was trained using weight percentage and temperature data at 5, 10, and 20  $^\circ\text{C min}^{-1}$ , and successfully predicted the decomposition profile at 15  $^\circ\text{C min}^{-1}$ . In addition, the activation energy of decomposition was determined using the Kissinger-Akahira-Sunose (KAS) method and incorporated into the ANN model to predict activation energy outputs. Model performance was optimized using the correlation coefficient (R) and mean squared error (MSE). The Bayesian Regularization (BR) and Levenberg-Marquardt (LM) algorithms yielded minimal errors: 0.01% and 0.04% for TG weight (%) predictions, and 0.15% and 5.79% for KAS activation energy (E<sub>a</sub>) values, respectively. These findings demonstrate that ANN can effectively predict the thermal decomposition behavior and activation energy of novel AP/LaMn<sub>0.4</sub>Fe<sub>0.6</sub>O<sub>3</sub> compositions under different heating rates, providing a valuable tool for the design of advanced propellant formulations.

**To be presented in  
Inorganic Chemistry Section**

**GLORIOUS RECORD OF ICC PAST CONFERENCES  
WITH SECTIONAL PRESIDENTS IN THEIR RESPECTIVE SECTIONS**

<b>Conf.</b>	<b>Date/Year</b>	<b>Local Organiser</b>
<b>1st</b>	<b>20–21 Sept., 1981</b>	<b>Indian Council of Chemists at Hotel Clarks Shiraz, Agra</b>
	Inorganic	Prof. T. N. Srivastava, Lucknow University, Lucknow
	Organic	Prof. P. R. Singh, IIT, Kanpur
	Physical	Prof. S. P. Srivastava, Roorkee University, Roorkee
<b>2nd</b>	<b>06–08 Nov., 1982</b>	<b>Kashmir University, Srinagar (J &amp; K)</b>
	Inorganic	Prof. M.M. Taqui Khan, Director, CSMCRI, Bhavnagar
	Organic	Prof. M. S. R. Naidu. S.V. University, Tirupati
	Physical	Prof. Aizaz Baig, Aligarh Muslim University, Aligarh
<b>3rd</b>	<b>28–30 Oct., 1983</b>	<b>Karnataka University, Dharwad</b>
	Inorganic	Prof. L. D. Dave, Bhavnagar University, Bhavagar
	Organic	Prof. P. R. Singh, IIT, Kanpur
	Physical	Prof. H. C. Gaur, Delhi University, Delhi
<b>4th</b>	<b>30–31 Dec., 1984 &amp; 1 Jan., 1985</b>	<b>Gorakhpur University, Gorakhpur</b>
	Inorganic	Prof. S. S. Sandhu, G.N.D. University, Amritsar
	Organic	Prof. S. C. Palerashi, Indian Institute of Chemical Biology, Jadavpur, Kolkata
	Physical	Prof. E. S. Jayadevappa, Karnataka University, Dharwad
	Anal.& Env.	Prof. S.G. Tandon, R.S. University, Raipur
<b>5th</b>	<b>27–29 Dec., 1985</b>	<b>Central Fuel Research Institute (CFRI), Sindri, Dhanbad</b>
	Inorganic	Prof. G.K.N. Reddy, Bangalore University, Bangalore
	Organic	Prof. D. Natsepuri, Indian Institute of Chemical Biology, Jadavpur, Kolkata
	Physical	Prof. M. L. Lakhadpal, Panjab University, Chandigarh
	Anal.& Env.	Prof. S.G. Tandon, R.S. University, Raipur
<b>6th</b>	<b>27–29 Dec., 1986</b>	<b>Madurai Kamraj University, Madurai</b>
	Inorganic	Prof. P. P. Singh, Bareilly College, Bareilly
	Organic	Prof. M. M. Bokadia, Vikram University, Ujjain
	Physical	Prof. Y. K. Gupta, Rajasthan University, Jaipur
	Anal.& Env.	Prof. S.M. Khopkar, IIT, Mumbai
	Bio-Chemistry	Prof. D.T. Jayaraman, Madurai Kamaraj Univ., Madurai



<b>7th</b>	<b>Dec., 1987</b>	<b>Jiwaji University, Gwalior</b>
	Inorganic	Prof. G. K. Chaturvedi, G. B. Pantnagar University, Pantnagar
	Organic	Prof. J. P. Saxena, Jodhpur University, Jodhpur
	Physical	Prof. B. Sethuram, Osmania University, Hyderabad
	Anal.& Env. Bio-Chemistry	Prof. Y.K. Agrawal, M.S. University, Baroda Prof. Rattan Singh, Punjab Agriculture Univ., Ludhiana
<b>8th</b>	<b>1988</b>	<b>Sri Venkateshwara University, Tirupati</b>
	Inorganic	Prof. D.V. Jahagirdar, Marathwada University, Aurangabad
	Organic	Prof. S. P. Hiremath, Gulbarga University, Gulbarga
	Physical	Prof. K. N. Mehrotra, Agra University, Agra
	Anal.& Env. Bio-Chemistry	Prof. B.K. Pal, Jadavpur University, Kolkata Prof. A.M. Siddiqui, Aligarh Muslim University, Aligarh
<b>9th</b>	<b>1990</b>	<b>Gulbarga University, Gulbarga</b>
	Inorganic	Prof. K. N. Munshi, Nagpur University, Nagpur
	Organic	Prof. J. N. Srivastava, Bhagalpur University, Bhagalpur
	Physical	Prof. R. C. Srivastava, B.H.U., Varanasi
	Anal.& Env. Bio-Chemistry	Prof. J. Rama Reddy, S.V. University, Tirupati Prof. T. Ramasarma, Indian Inst. of Science, Bangalore
<b>10th</b>	<b>28–30 Oct., 1991</b>	<b>Goa University, Goa</b>
	Inorganic	Prof. M. L. Dhar, Jammu University, Jammu
	Organic	Prof. G. K. Trivedi, IIT, Mumbai
	Physical	Prof. P. C. Nigam, Manipur University, Imphal
	Anal.& Env.	Prof. S.N. Tandon, Roorkee University, Roorkee
<b>11th</b>	<b>12–14 Mar., 1993</b>	<b>Bihar University, Muzaffarpur</b>
	Inorganic	Prof. K. C. Satpathy, Sambhalpur University, Burla
	Organic	Prof. V. K. Saxena, Dr. H.S. Gaur University, Sagar
	Physical	Prof. K. C. Nand, Jiwaji University, Gwalior
	Anal.& Env.	Prof. K.G. Varshney, Dr. Z.H. College of Engg. & Tech., Aligarh
<b>12th</b>	<b>Dec., 1993</b>	<b>Kakatiya University, Warangal</b>
	Inorganic	Prof. A. S. R. Murthy, Andhra University, Guntur
	Organic	Prof. D. Bhaskar Reddy, S.V. University, Tirupati
	Physical	Prof. S. I. Ali, Jamia Millia Islamia, New Delhi
	Anal.& Env.	Prof. B.M. Schinde, Inst. of Science, Mumbai
<b>13th</b>	<b>1994</b>	<b>Jammu University, Jammu (J &amp; K)</b>
	Inorganic	Prof. R. R. Naidu, S. V. University, Tirupati
	Organic	Prof. S. C. Sharma, H.P. University, Shimla
	Physical	Prof. R. K. Prasad, L. S. College, Muzaffarpur
	Anal.& Env.	Prof. P.A. Puja, Gulbarga University, Gulbarga

<b>14th</b>	<b>28-30 Dec., 1995</b> Inorganic Organic  Physical Anal.& Env.	<b>The Institute of Science, Mumbai</b> Prof. N. K. Jha, IIT, Delhi Prof. S. Shivasubramanian, Madurai University, Madurai Prof. N. K. Sharma, University of Jammu, Jammu Prof. R.T. Sane, R.H. Ruia College, Mumbai
<b>15th</b>	<b>24-26 Oct., 1996</b> Inorganic Organic  Physical Anal.& Env.	<b>Dr. B.R. Ambedkar University, Aurangabad (M.S.)</b> Prof. P. G. Ramappa, Mysore University, Mysore Prof. P. S. Kalsi, Punjab Agricultural University, Ludhiana Prof. V. Ananta Raman, Andhra University, Vishakhapatnam Prof. S.P. Mathur, M.D. University, Ajmer
<b>16th</b>	<b>Oct., 1997</b> Inorganic Organic Physical Anal.& Env.	<b>Mangalore University, Mangalore</b> Prof. K. C. Patel, Indian Institute of Science, Bangalore Prof. S. Y. Ambekar, Mysore University, Mysore Prof. S. C. Ameta, M. L. Sukhadia University, Udaipur Prof. Mrs. S.K. Menon, Gujarat University, Ahmedabad
<b>17th</b>	<b>26-28 Nov., 1998</b> Inorganic Organic Physical Anal.& Env.	<b>Madras University, Chennai</b> Prof. S. F. Patil, North Maharashtra University, Jalgaon Prof. A. K. Singh, IIT, Mumbai Prof. Bharat Singh, Allahabad University, Allahabad Prof. T.S. Pal, IIT, Kharagpur
<b>18th</b>	<b>27-29 Dec., 1999</b> Inorganic Organic Physical Anal.& Env.	<b>North Maharashtra University, Jalgaon</b> Prof. M. C. Chakraborty, IIT, Kharagpur Prof. M. M. Salunkhe, Institute of Science, Mumbai Prof. (Mrs) Surekha G. Devi, M. S. University, Baroda Prof. S.M. Khopkar, IIT, Mumbai
<b>19th</b>	<b>27-29 Nov., 2000</b> Inorganic Organic Physical Anal.& Env.	<b>Kuvempu University, Shimoga</b> Prof. R. C. Maurya, R. D. University, Jabalpur Prof. (Mrs.) Sujata V. Bhat, IIT, Mumbai Prof. B. Thimme Gowda, Mangalore Univ., Mangalore Prof. V.K. Gupta, R.S. University, Raipur
<b>20th</b>	<b>22-24 Dec., 2001</b> Inorganic Organic Physical Anal.& Env.	<b>Mysore University, Mysore</b> Prof. B. L. Khandelwal, D.M.S.R.D.E., Kanpur Dr. V. S. Ekkundi, CIBA India Pvt. Ltd., Mumbai Prof. M. K. Mishra, IIT, Mumbai Prof. Syed Akeel Ahmad, Mysore University, Mysore
<b>21st</b>	<b>24-26 Oct., 2002</b> Inorganic Organic Physical Anal.& Env.	<b>Rani Durgavati University, Jabalpur (M.P.)</b> Prof. P. K. Bhattacharya, M.S. University, Baroda Prof. H. M. Chawla, IIT, New Delhi Prof. B. L. Thembe, IIT, Mumai Prof. K.K. Verma, R.D. University, Jabalpur

<b>22nd</b>	<b>17-19 Oct., 2003</b> Inorganic Organic Physical Anal.& Env.	<b>Indian Institute of Technology, Roorkee</b> Prof. Ranjeet K. Verma, Magadh University, Bodh-Gaya Prof. S. S. Talwar, IIT, Mumbai Prof. A. K. Jain, IIT, Roorkee Prof. P.K. Padmanabhan, BARC, Mumbai
<b>23rd</b>	<b>29-31 Oct., 2004</b> Inorganic Organic  Physical Anal.& Env.	<b>K.C. College, Churchgate, Mumbai</b> Prof. Lallan Mishra, B. H. U., Varansi Prof. N. S. Prakasa Rao, Nagarjuna University, Nagarjunanagar Prof. S. K. Dogra, IIT, Kanpur Prof. K.S. Pitre, Dr. H.S. Gaur Univ., Sagar
<b>24th</b>	<b>16-18 Dec., 2005</b> Inorganic  Organic Physical Anal.& Env.	<b>Birla Institute of Technology, Mesra, Ranchi</b> Prof. S. K. Roy, Vinoba Bhave University, Hazaribagh (Jharkhand) Prof. K. R. Desai, South Gujrat University, Surat Prof. Girjesh Govil, TIFR, Mumbai Prof. Kaza Somasekhara Rao, Acharya Nagarjuna Univ., Nuzvid
<b>25th</b>	<b>27-29 Dec., 2006</b> Inorganic Organic Physical Anal.& Env.  Pharmaceutical	<b>Birla College of Arts, Science &amp; Com., Kalyan (M.S.)</b> Prof. R. C. Srivastava, Lucknow University, Lucknow Prof. K. S. Rangappa, Mysore University, Mysore Prof. M. K. Mahanti, North-Eastern Hill Univ., Shillong Prof. H.S. Rathore, Z.H. College of Engg. & Tech., AMU, Aligarh Prof. Anamik Shah, Saurashtra University, Rajkot
<b>26th</b>	<b>26-28 Feb., 2008</b> Inorganic Organic Physical  Anal.& Env. Pharmaceutical	<b>Dr. H.S. Gour University, Sagar (M.P.)</b> Prof. P. Indrasenan, Univ. of Kerala, Tiruvanthapuram Prof. S. Kabilan, Annamalai University, Annamalaiagar Prof. Ashok Kumar Sharma, Devi Ahilya University, Indore Prof. A.D. Sawant, Mumbai University, Mumbai Dr. P.M.S. Chauhan, CDRI, Lucknow
<b>27th</b>	<b>26-28 Dec., 2008</b> Inorganic Organic  Physical Anal.& Env. Pharmaceutical	<b>Gurukul Kangri Vishwavidyalaya, Haridwar</b> Prof. C. P. Bhasin, HNG University, Patan Prof. Balakrishna Kalluraya, Mangalore University, Mangalore Dr. L. Gomithi Devi, Bangalore Univ., Bangalore Dr. Rakesh Kumar, NEERI, Worli, Mumbai Prof. M.P.S. Ishar, Gurunanak Dev University, Amritsar

<b>28th</b>	<b>07-10 Nov., 2009</b> Inorganic Organic  Physical Anal.& Env.  Pharmaceutical	<b>Hem North Gujarat University, Patan (Gujarat)</b> Dr. A. S. Aswar, SGB Amravati University, Amravati Prof. B. H. M. Mritunjaya Swami, Gulbarga University, Gulbarga Prof. A. K. Srivastava, Allahabad Univ., Allahabad Prof. G. Rama Krishna Naidu, Sri Venkateswar University, Tirupati Prof. C.S. Mahela, Kumaun University, Nainital
<b>29th</b>	<b>19-21 Dec., 2010</b> Inorganic Organic Physical Anal.& Env. Pharmaceutical	<b>Panjab University, Chandigarh</b> Prof. A. K. Manihar Singh, Manipur University, Imphal Prof. D. Ashok, Osmania University, Hyderabad Prof. S. T. Nandibewoor, Karnatak University, Dharwad Prof. K.S. Gupta, University of Rajasthan, Jaipur Prof. M. Himaja, VIT University, Vellore
<b>30th</b>	<b>28-30 Dec., 2011</b> Inorganic Organic  Physical Anal.& Env. Pharmaceutical	<b>Osmania University, Hyderabad</b> Prof. A. K. Singh, IIT, Delhi Prof. M. V. Basaveswara Rao, Krishna University, Machilipatnam, A.P. Prof. S. A. Chimatadar, Karnataka Univ., Dharwad Prof. A.K. Singh, IIT, Delhi Dr. P.M.S. Chauhan, CDRI, Lucknow
<b>31st</b>	<b>26-28 Dec., 2012</b> Inorganic Organic Physical Anal.& Env. Pharmaceutical	<b>Saurashtra University, Rajkot</b> Prof. H. P. S. Chauhan, Devi Ahilya University, Indore Prof. N. C. Desai, M.K. Bhavnagar Univ., Bhavnagar Prof. S. K. Mehta, Panjab Univ., Chandigarh Prof. I. Ajit Kumar Reddy, NIT Warangal Prof. Naveen B. Patel, VNSG University, Surat
<b>32nd</b>	<b>28-30 Nov. 2013</b> Inorganic Organic Physical Anal.& Env. Pharmaceutical	<b>Karnataka University, Dharwad</b> Prof. A. P. Mishra, H. S. Gour University, Sagar Prof. D. Channe Gowda, Mysore University, Mysore Prof. M. B. Halli, Gulbarga Univ. Gurbarga Prof. J.J. Vora, H.N.G. University, Patan Dr. Anil Kumar Dwivedi, CDRI, Lucknow
<b>33rd</b>	<b>15-17 Dec., 2014</b> Inorganic Organic Physical Anal.& Env. Pharmaceutical	<b>Indian School of Mines, Dhanbad</b> Prof. Shivraj, Osmania University, Hyderabad Prof. C. Venkata Rao, Sri Venkateswara Univ., Tirupati Prof. M. M. Singh, BHU, Varanasi Prof. Sanjoy Mishra, Ranchi University, Ranchi Prof. N.S. Rajurkar, Pune University, Pune
<b>34th</b>	<b>26-28 Dec., 2015</b> Inorganic Organic Physical Anal.& Env. Pharmaceutical	<b>UKA Tarsadia University, Bardoli, Surat</b> Prof. D. D. Pathak, ISM, Dhanbad Prof. Kotha Sambasiva Rao, IIT Bombay Prof. Ali Mohammad, AMU, Aligarh Dr. V.S. Srivastava, G.T.P. College, Nandurbar Prof. Shailesh Shah, UKA Tarsadiya Univ., Bardoli, Surat

<b>35th</b>	<b>22-24 Dec., 2016</b>  Inorganic Organic  Physical Anal.& Env. Pharmaceutical	<b>Haribhai V. Desai College Pune &amp; College of Engg., Pune</b> Dr. R. K. Agrawal, Lajpat Rai P.G. College, Sahibabad Prof. Balakrishna Kalluraya, Mangalore University, Mangalore Prof. R. Sambasiva Rao, Andhra Univ., Visakhapatnam Prof. S.K. Pardeshi, Pune University, Pune Prof. K. Sathiyararayana, VIT University, Vellore
<b>36th</b>	<b>26-28 Dec., 2017</b>  Inorganic Organic  Physical Anal.& Env. Pharm. & Bio-Chemistry	<b>Andhra University, Visakhapatnam</b> Prof. Sushil K. Pandey, University of Jammu, Jammu Prof. Vommima V. Sureshbabu, Bangalore Univ., Bangalore Prof. Krishnaiah Abburi, Tirupati Prof. Prafulla K. Sahoo, Utkal University, Bhubaneswar Prof. P. Vani, Andhra University, Visakhapatnam
<b>37th</b>	<b>12-14 Dec., 2018</b>  Inorganic Organic Physical Anal.& Env. Pharm. & Bio-Chemistry	<b>National Institute of Technology Karnataka, Surathkal, Karnataka</b> Prof. B. Narayana, Mangalore University, Mangalore Prof. J. J. Vora, HNG University, Patan Prof. Puttaswami, Bangalore Univ., Bangalore Prof. R.K. Dubey, Allahabad University, Allahabad Prof. J. Saravanan, PES College of Pharmacy, Bangalore
<b>38th</b>	<b>26-28 Dec., 2019</b> Jaipur Organic  Physical Anal.& Env. Pharm. & Bio-Chemistry	<b>Jaipur National University, Jaipur</b> Prof. B. K. Rai, Muzaffarpur Prof. Bhaskar S. Dawane, Marathwada University, Nanded Prof. Harsh Manchanda, NIT, Jalandhar Prof. Pradeep Kumar Sharma, J.N.V. Univ., Jodhpur Prof. D. Ashok, Osmania University, Hyderabad
<b>39th</b>	<b>10-11 Apr., 2021</b> (Online) Inorganic Organic Physical Anal.& Env. Pharma.	<b>Veer Narmad South Gujarat University, Surat</b> Prof. R. N. Patel, A.P.S. University, Rewa Prof. M. Vijulatha, Osmania University, Hyderabad Prof. Amalendu Pal, Kurukshetra Univ., Kurukshetra Prof. Pranav Srivastava, Gujarat Univ. Ahmedabad Prof. K.H. Chikhalia, VNSG University, Surat
<b>40th</b>	<b>29-30 Dec., 2021</b> (Online) Inorganic Organic  Physical Anal.& Env. Pharma.	<b>Satavana University, Karimnagar, Telangana</b> Prof. Shivadhar Sharma, Magadh University, Bodh-Gaya Prof. Panaganti Leelavathi, Osmania University, Hyderabad Prof. Pannuru Venkatesu, University of Delhi, Delhi Prof. Satish K. Pardeshi, S.P. Pune University, Pune Dr. Hitesh D. Patel, Gujarat Univ., Ahmedabad

<b>41st</b>	<b>27-29 Dec., 2022</b>  Inorganic Organic Physical Anal.& Env.	<b>Institute of Basic Sciences, Dr. B. R. Ambedkar University, Agra</b> Dr. Abhay Nand Sahay, TM Bhagalpur Univ., Bhagalpur Prof. A. Jaya Shree, J.N. Technological Univ., Hyderabad Prof. P. Venkatesu, Delhi University, Delhi Dr. A.S. Aswar, S.G.B. Amravati University, Amravati
<b>42nd</b>	<b>20-22 Dec., 2023</b>  Inorganic Organic Physical  Anal.& Env.	<b>University of Kota, Kota, Rajasthan</b> Prof. G. S. Gugale, H. V. Desai College, Pune Prof. Kishore Chikhalia, VNSG University, Surat Prof. Pradeep K. Sharma, JNV, Jodhpur in place of Prof. M.Y. Karidurganavar, Karnatak Univesity, Dharwad Prof. Jaya Dwivedi, Banasthali University, Banasthali
<b>43rd</b>	<b>26-28 Dec., 2024</b>  Inorganic  Organic Physical Anal.& Env.	<b>Modern College of Arts, Science &amp; Commerce, Pune &amp; H. V. Desai College, Pune</b> Prof. R. N. Patel, Rewa in place of Dr. R. N. Jadeja, M. S. University, Baroda Prof. Beeraiah Baire, IIT Madras, Chennai Prof. Dilip H. Dagade, Shivaji Univ., Kolhapur Prof. Tamal Banerjee, IIT,Guwahati
<b>44th</b>	<b>22-24 Dec., 2025</b>  Inorganic Organic Physical Anal.& Env.	<b>KLE Technological Univ., Hubballi, Karnataka</b> Prof. V. K. Sharma, Lucknow University, Lucknow Prof. Arun M. Isloor, NIT Karnataka, Surathkal Prof. Ramesh L. Gardas, IIT Madras, Chennai Prof. Annamalai Senthil Kumar, Vellore Institute of Technology University, Tamil Nadu

**SYMPOSIUM ON  
“RECENT ADVANCES IN POLYMER SCIENCE  
AND TECHNOLOGIES - EMERGING  
MULTIFUNCTIONAL POLYMERIC MATERIALS”**

**Sectional President's Address**

**Polymeric Materials in Health, Energy and Environment**

**Tejraj M. Aminabhavi**

*Center for Energy and Environment, School of Advanced Sciences, KLE  
Technological University, BVBCET Campus, Hubballi 580031, Karnataka  
E-mail: aminabhavit@kletech.ac.in*

Development of new polymers and materials required in industrial sectors for environmental applications, membrane separations and biomedical areas are being actively pursued over many decades. Among the polymeric materials that deserve to be highlighted as different types of polymers and materials for the benefit of mankind such as adsorption of contaminants (pesticides, potentially toxic metals, and medicines, among others) to provide clean environment for health benefits. Photocatalytic polymers and materials, surface coatings without the degradation of organic compounds in water, polymeric membranes used for filtration of toxic contaminants in water media for the restoration of ecosystems and release of specific compounds, biodegradable plastics for renewable resources and conducting polymers in renewable energy storage and energy production areas as well developing polymers in biomedical fields such as drug delivery systems, targeted therapy, scaffolds in tissue engineering, implantation of medical device artificial organs, prosthesis, ophthalmology, dentistry, bone repair, and many other medical fields are the outcomes of research efforts around the world. Owing to good biocompatibility and easy modification, natural polymers are now a great interest in biomedical applications. Similar efforts are being pursued in developing novel materials required in energy production technologies. Representative examples of these areas are covered briefly. Managing plastic waste is one of the major concerns worldwide as it impacts the

environment and releases pollutants and toxic chemicals<sup>1</sup>. In particular, multi-layered plastic (MLP) is one of the categories which is widely used in the food and packaging industries. MLP packaging is generally made from 3-7 thin layers consisting of aluminum foil with a cascade of paper polyethylene (PE), polyethylene terephthalate (PET), polypropylene (PP), polyamide (PA), polystyrene (PS), polyvinylchloride (PVC). Upcycling/recycling of MLPs has been reported in recent studies utilizing primary recycling: mechanical recycling, secondary recycling: solvolysis/chemical and tertiary recycling: pyrolysis/energy recovery. The low recycling rate, energy consumption, CO<sub>2</sub> emissions, and consumption of a lot of chemicals are the problems associated with chemical and mechanical treatments. Solvent-targeted recovery and precipitation is an emerging technology for deconstructed into their constituent resins before being co-fed into processing equipment to produce reconstituted multilayer films, but it still, has a long way to become commercially viable technologies. A thermal treatment especially using pyrolysis wherein polyolefins are decomposed at an elevated temperature of 400-500 °C in the absence of oxygen.



## **PSIL-01: Bio - Compostable Plastics - Redefining Sustainability for Circular Economy**

**Virendrakumar Gupta**

*Reliance Research and Development Centre, Reliance Industries Limited, Navi Mumbai 400701, Maharashtra*

*E-mail: Virendrakumar.Gupta@ril.com*

Bio-Compostable Plastic, Polybutylene adipate terephthalate (PBAT), is an important class of compostable polyesters. It has flexibility, toughness, and good processability, such properties, make PBAT a sustainable alternative to conventional plastics like polyolefins. Chemically PBAT is a random aliphatic-aromatic copolyesters and a range of products can be made of this for single-use applications. PBAT has ability to biodegrade under industrial composting conditions. Moreover, PBAT properties can be enhanced by blending it with other compostable plastics such as PLA, PBS, PHA and natural polymers such as starch and fibres. PBAT based bioplastics offers a promising pathway for circular economy model through plastic waste reduction. The present talk will focus on PBAT's distinctive role as a compostable polymer and highlights PBAT-composite-based packaging for single-use products.

## **PSIL-02: Recycling of Waste Plastics into Hydrocarbons - The Circular Economy**

**Anand B. Halgeri**

*Poornaprajna Institute of Scientific Research, Bengaluru 562110, Karnataka*

*E-mail: abhalgeri@gmail.com*

Ever-increasing consumption of Plastic Products and poor waste management have resulted in massive accumulation of plastic waste in the environment, causing adverse effects on the climate and living organisms. Although contributing 10% towards the total waste management infrastructure, the chemical recycling of waste plastics is a considerably viable option to valorise waste into platform chemicals and liquid fuel. Several chemical processes are being used, including Mechanical Mixing of Waste plastics, reprocessing of used plastics, and pyrolysis at very elevated temperatures produce hydrocarbons. Chemical Recycling can convert plastic waste into higher-value products, such as liquid fuels, platform chemicals, and virgin plastics. Various chemical recycling approaches, including pyrolysis, gasification, hydrogenolysis, solvolysis, and cracking. Pyrolysis and Gasification at higher temperatures, whereas Catalytic hydrogenolysis and hydrocracking operate under milder conditions than pyrolysis, offering higher selectivity to hydrocarbons and value products. The present deals with the design and development of zeolite-

based Catalysts for the conversion of Waste plastics into fuel-grade oil. A detailed study has been undertaken on the modification. Zeolite Catalyst and Characterisation to get the higher selectivity of desired products. Optimisation of process parameters and recyclability of Catalysts have been extensively carried out. The study highlights a low-temperature strategy, contributing to energy efficiency and plastic waste mitigation. The entire know-how was transferred to Ms Thermax Pune for the fabrication of the prototype machine, which may be useful in an urban complex for handling plastic waste on-site demand. The talk will also highlight a comparative study of technological advancement in the pyrolysis of Waste Plastics, both in India and abroad

### **PSIL-03: Design and Syntheses of Well-Defined Functional Macromolecular Architectures from Controlled Radical Polymerization: Role in Various Applications**

**Annadanam V. Sesha Sainath**

*Fluoro-Agrochemicals, Polymers and Functional Materials Department, CSIR-Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad 500007, Telangana*  
*E-mail: avssainath@yahoo.com avss.iict@csir.res.in*

Polymer science and engineering play a pivotal role in the creation of value-added materials that support modern technological advancements. Our research group focuses on the design and synthesis of multi-component macromolecular architectures with specific functional groups through tailored approaches. Our group has developed a diverse range of monomers with various functional moieties and constructed well-defined macromolecular architectures using advanced controlled radical polymerization techniques. These include iniferter (initiator, transfer agent, and terminator), ATRP (atom transfer radical polymerization), and RAFT (reversible addition–fragmentation chain transfer) methods. Additionally, we investigate macromolecular terminal end functionalization and its application in initiating monomers to achieve precisely engineered polymer structures. In this talk, we present our past and present research on the design and synthesis of novel glyco-, fluoro-, and electron-rich monomers, as well as their corresponding macromolecular architectures. These innovations have driven significant technological advancements and helped a diverse array of practical applications across multiple fields. We discuss how the structural features of the macromolecular chains contribute to a fundamental understanding of the functional pendant moieties present

in the polymer segments for various applications (Figure 1). For instance, the PEO-based diblock copolymer exhibits self-assembled morphologies in thin films, which can act as nano-reactors. Membranes fabricated from ABA triblock copolymer and PVDF blends demonstrated approximately 2.5 times higher water flux and 99% oil rejection at an operating pressure of 2 bar for engine oil–water emulsion feeds, compared to neat PVDF membranes. Furthermore, the synthesized hydrophilic polymer architectures were utilized to investigate their roles in photocatalytic  $H_2$  production using various photocatalysts. We developed several block copolymers, including polystyrene-*b*-poly(methacryloyl-D-glucose), fluoro-segmented glycopolymer (PPFBM-*b*-PGD), poly(4-vinylpyridine)-*b*-poly(methacryloyl-D-glucose) (an electron-rich pyridine-based copolymer), and a cobaloxime catalyst  $[Co(dmgh_2)(dmgh)Cl_2]$  incorporated into a pyridine-based homopolymer (P4VP-Co). Interestingly, the developed metal chelated polymer achieved an  $H_2$  evolution rate of 4299  $\mu\text{mol/h/g}$ . In my presentation, I will discuss the photoreforming mechanism and how macromolecular architecture influences  $H_2$  production. While macromolecular architectures offer significant potential as viable technologies, challenges remain, including the fixation of functional groups within the macromolecular chain, stability issues, high costs, and limitations in polymer synthesis. Addressing these challenges through targeted engineering approaches is essential for advancing macromolecular synthesis for targeted applications.

## **PSIL-04: The Unbreakable Solution: Vitrimers for a World Without Polymer Waste**

**Suryasarathi Bose**

*Department of Materials Engineering, Indian Institute of Science, Bengaluru  
560012, Karnataka  
E-mail: sbose@iisc.ac.in*

The research in my group is dedicated to advancing the Circular Economy through innovative polymer chemistry and materials engineering. We focus on two critical areas: the upcycling and chemical recycling of high-volume commodity thermoplastics (Polypropylene, Polyethylene, Polystyrene, Polyamides, and ABS), and the design of novel, re-processable thermosets. Our central innovation lies in synthesizing vitrimers from both traditionally intractable thermosets and commodity thermoplastics by incorporating unique Dynamic Covalent Adaptable Networks (CANs). This strategy enables materials to be reshaped, repaired, and recycled without compromising performance. Specific outcomes include the development of bio-based vitrimers and scalable methods, such as the SaLSO™ protocol, which

transform low-value waste into high-performance feedstocks. This work establishes molecular-level solutions to achieve sustainable manufacturing and resource circularity.

## **PSIL-05: Transforming Industry and Society Through Advanced Membrane Solutions**

**S. Sridhar**

*Chemical Engineering and Process Technology Department, CSIR-Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad 500007, Telangana  
E-mail: sridhar11in@yahoo.com*

Membrane technology has evolved rapidly across industries, offering advantages such as enhanced process safety, environmental sustainability, and reduced capital and operating costs. This work presents the development of innovative membranes and integrated processes for diverse industrial and societal applications. Case studies demonstrate their effectiveness in tackling environmental pollution and other global challenges. Laboratory-scale studies on olefin–paraffin separations using advanced silver-incorporated membranes show significant potential to reduce refinery energy consumption. A hybrid electrodialysis–distillation process was developed to treat pharmaceutical effluents, enabling the recovery of 30 MT of DMSO for antiretroviral drug synthesis while isolating hazardous salts. Additional membrane applications include zero-liquid discharge (ZLD) treatment of effluents from acrylic fiber, aromatics, and coke oven industries. Fuel cell membranes were also designed as zero-emission alternatives. India’s first gas separation pilot plant, established at ONGC’s Hazira facility, demonstrated reduced reliance on polluting amine-based solvents. A cascaded RO–resin hybrid system was engineered to produce ultrapure water for hospitals and research laboratories, benefitting over 200,000 dialysis patients. Indigenous, low-cost hemodialysis membranes are currently under development, with promising laboratory results for efficient uremic toxin removal and strong commercialization prospects. To address water scarcity, CSIR-IICT developed Atmospheric Water Generators and defluoridation/nanofiltration systems that now serve over five million people in water-stressed terrains, and regions affected by fluorosis, jaundice, cholera and other water-borne diseases. Portable hand-pump filtration units were deployed in flood-affected areas to provide safe drinking water. In CSIR-IICT campus, over 30 pilot and tabletop membrane units operate daily, supplying potable to the staff, and students besides and ultrapure medical-grade water for laboratory applications. During the COVID-19 pandemic, the institute developed multilayer masks, face shields, touch-free sanitizing systems, and ultrapure water units

for sanitizer production. Over six lakh masks and 2,000 shields were distributed across 20 states, generating Rs. 2 crore in revenue and creating employment for 500 women and senior citizens. Other healthcare innovations included UV disinfection chambers, alkaline water devices, and emergency ventilators. Future research aims to advance solvent recovery from refinery wastewater and scale up indigenous membrane technologies for electrolyzers, pervaporation, gas separation, and solar-powered desalination.

## **PSIL-06: Smart Anisotropic Colloidal Composites: A Novel Platform for Modifying the Phase Transition of Diblock Copolymer by Gold Nanoparticles**

**Pannuru Venkatesu**

*Department of Chemistry, University of Delhi, Delhi-110 007*

*E-mail: pvenkatesu@chemistry.du.ac.in*

Surface modification of metallic nanoparticles (NPs) by stimuli responsive polymers (SRPs) is a benign method to prepare smart colloidal composites which tunes the characteristic properties of individual systems. The temperature dependent transition of diblock copolymer poly(N-isopropylacrylamide)-block-poly(N-vinylcaprolactam) (PNIPMA-b-PVCL) synthesized using reversible addition-fragmentation chain transfer (RAFT) polymerization and was studied by incorporating anisotropic gold nanoparticles (AGPs) such as spheres (AuNSs), rods (AuNRs), cubes (AuNCs) and rhombic dodecahedrals (AuRDs). Shape dependent physiochemical properties of nanostructures alter the lower critical solution temperature (LCST) of chemical inhomogeneous diblock copolymer. Heterogeneous nucleation of AuNPs was facilitated by seed mediated synthesis for incorporating uniformity. In the mixed system, presence of PNIPAM-b-PVCL modifies the surface of AGPs through physisorption which is supported by transmission electron microscopy (TEM) and field emission scanning electron microscopy (FESEM) showing the nanoparticles embedding in the polymeric matrix. Steady state fluorescence spectroscopy and Fourier transform infrared spectroscopy (FTIR) were performed to examine the interactions between AGPs and PNIPAM-b-PVCL. Formation of smart polymer nanocomposite alters the physiochemical properties of diblock copolymer as demonstrated from the variation of LCST in dynamic light scattering (DLS) measurement. Henceforth, functionalizing the surfaces of AGPs with thermoresponsive diblock copolymer provides combinatorial benefits in properties of smart polymeric colloidal systems with potential application in bioimaging, and surface enhanced Raman Scattering (SERS).

## ANALYTICAL AND ENVIRONMENTAL CHEMISTRY SECTION

### Sectional President's Address

#### **Redox-Active Organic Molecular Species Anchored Carbon Nanomaterials for Elegant Electrochemical Immunoassays**

**Annamalai Senthil Kumar**

*Nano and Bio-electrochemistry Research Laboratory, Department of Chemistry,  
School of Advanced Sciences and CO<sub>2</sub> Research and Green Technology Centre,  
Vellore Institute of Technology University, Vellore-632 014, Tamil Nadu  
E-mail : askumarchem@yahoo.com askumar@vit.ac.in*

Electrochemical immunosensors are powerful tools for rapid, sensitive, and selective biomolecule detection, as they combine antigen–antibody specificity with reliable electrochemical readouts. Carbon-based nanomaterials such as carbon nanotubes, graphene, and mesoporous carbons are key components in these devices because their high conductivity and large surface area enable efficient electron transfer and high loading of biorecognition elements. Traditional immunosensors often use solution-phase redox probes like ferricyanide, but these can generate false-positive signals and reduce accuracy. To overcome this, our research group has focused on immobilizing redox-active organic molecules directly onto carbon nanomaterials, creating more stable and dependable signal interfaces. For example, we developed a UPEC (*E. coli*) immunosensor by anchoring the redox dye Thionine (Th) onto a functionalized MWCNT–chitosan matrix on a glassy carbon electrode. Stepwise assembly of the target bacteria, blocking agents, primary antibodies, and HRP-labeled secondary antibodies produced a robust sandwich immunoassay with a clear and sensitive redox response. The same design principles were successfully used for detecting human serum albumin and malarial protein biomarkers. These results demonstrate the strong synergy between conductive carbon scaffolds and surface-bound organic redox mediators,

leading to stable, versatile, and high-performance immunosensing platforms. Such systems offer tunable redox properties, improved selectivity, and adaptable sensor designs suitable for detecting various pathogens and disease biomarkers, with promising potential for point-of-care testing. Despite these advances, challenges remain: improving mediator stability, preventing leaching, reducing nonspecific adsorption, and ensuring reproducible electrode fabrication, especially for real-sample analysis. My presentation will discuss our recent progress in functionalizing carbon nanomaterials with redox-active organic molecules and highlight strategies for developing next-generation electrochemical immunosensors with enhanced sensitivity, stability, and practical usability.



## AEIL-01 : Technology Readiness and Innovation Gaps in Electrolyzers for Green Hydrogen

Ujjwal Pal

*Department of Energy and Environmental Engineering, CSIR-Indian Institute of Chemical Technology, Hyderabad, 500007*

*E-mail : [ujjwalpal@iict.res.in](mailto:ujjwalpal@iict.res.in); [upal03@gmail.com](mailto:upal03@gmail.com)*

The next generation of alkaline water-splitting systems is expected to witness the breakthrough concept of decoupled electrolysis, wherein the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) are spatially or temporally separated to enhance flexibility, safety, and compatibility with intermittent renewable power. Recent advances in decoupled device architectures (e.g., split-cell, swing-cycle, or redox-mediator configurations) demonstrate the potential for lower cell voltages, improved durability, and simplified gas management. We report a hybrid membrane-free cell based on earth-abundant materials that enables decoupled hydrogen production in either acidic or alkaline medium. The design combines the electrocatalytic reactions of an electrolyzer with a capacitive storage mechanism, allowing spatial and temporal separation of hydrogen and oxygen evolution. Cell-voltage breakdown reveals that substantial improvements can be achieved by tuning the bifunctional catalyst activity and enhancing electrode conductivity, offering increased flexibility and robustness for sustainable hydrogen production. In this talk, we discuss how hybrid decoupled architectures integrated with Ni-Fe-based catalysts can address major limitations of conventional alkaline systems—such as gas crossover, restricted dynamic response, and catalyst degradation—while outlining a ten-year project roadmap. We further identify critical innovation gaps—from scaling bifunctional catalysts on industrial electrodes to ensuring long-term durability and integrating decoupled designs with redox or supercapacitive mediators. A forward-looking technology roadmap (2025–2035) is outlined: near-term targets emphasize pilot-scale (~100 kW) decoupled alkaline modules using Ni-Fe-based bifunctional catalysts and hybrid capacitive electrodes; mid-term objectives focus on gigawatt-scale commercialization, achieving cell voltages  $< 1.6$  V at  $500 \text{ mA cm}^{-2}$  and stack lifetimes  $> 40,000$  h, while maintaining adaptability to renewable intermittency.

If realized, this convergence of membrane-free decoupled electrolysis and modified bifunctional Ni-Fe based catalysis establishes a practical pathway toward low-cost, flexible, and scalable green hydrogen production.



## **AEIL-02 : Exploring Biodiversity for Energy and Environmental Applications**

**S.K. Nataraj**

*Centre for Nano & Material Sciences, JAIN University, Jain Global Campus, Bangalore- 562112*

*E-mail : sk.nataraj@jainuniversity.ac.in; sknata@gmail.com*

Major contributors to this include crop residues such as rice husks, wheat straw, and corn stover, all of which possess substantial cellulose content. Utilizing this abundant waste not only alleviates environmental challenges related to disposal but also provides a renewable and sustainable feedstock for extracting various chemicals and functional materials. We at Sustainable Materials and Processes Lab develop various protocols, methods and approach that offers an eco-friendly alternative to generate new functional and platform chemicals following sustainable resource management practices while advancing the development of bio-based materials for a wide range of industrial applications, including water filtration, energy conversion, energy storage, packaging and so on. The versatility of extraction steps developed, particularly chemicals like cellulose from agri-biomass, allows for its effective integration into membrane technology, energy storage devices and protein packaging. Their inherent hydrophilicity, mechanical strength, and antifouling properties significantly improve membrane performance in various separation processes and as polymer matrix allows the easy modification of functionality that is suitable for energy conversion and storage applications. These attributes make agro-biomass a key resource for material extraction with environmentally friendly and sustainable systems, especially for water treatment, energy storage, protein packing and other critical applications. Consequently, the use of vast agro biowaste not only promotes sustainability but also contributes to advancements in eco-efficient technologies across multiple sectors.

## **AEIL-03: The Chemical Language of Air: Analytical Stories from the Atmosphere**

**Ranjit Kumar**

*Department of Chemistry, Faculty of Science, Dayalbagh Educational Institute (Deemed University), Dayalbagh, Agra-5*

*E-mail: rkschem@rediffmail.com*

The atmosphere carries a quiet language of molecules, a shifting script written by natural processes, human activity, and the chemistry that links them. Modern analytical tools now allow us to read this language with greater clarity, revealing stories about sources, transformations, and the evolving state of air quality. This talk

examines how cutting-edge equipment, like as satellite retrievals, mobile sensor networks, high-resolution mass spectrometry, and cavity-enhanced spectroscopy, can reveal the chemical fingerprints that mold the air we breathe. These instruments reveal the delicate interactions between radicals, oxidants, and trace gases that control atmospheric reactivity, decipher the production of secondary pollutants, and monitor the aging of aerosols as they move across geographical boundaries. Urban canyons, rural fire plumes, and coastal interfaces are all included in the story, each of which has its own chemical lexicon. We can learn more about pollution episodes, cycles of diurnal transition, and uncommon occurrences that uncover hidden channels by piecing together evidence from various sizes. This talk's main objective is to demonstrate how analytical chemistry turns the atmosphere from a far-off background into an accessible record of events, influences, and patterns. In addition to offering scientific depth, an understanding of this chemical language serves as a roadmap for creating well-informed, practical plans to safeguard public health and air quality.

#### **AEIL-04: Advances in Hybrid nano-adsorbent and Nanofiltration Strategies for Safer and Sustainable Water Systems**

**Raviraj M. Kulkarni**

*School of Computing, MIT Vishwaprayag University, Solapur 413255, Maharashtra*

*E-mail: ravirajmkulkarni@gmail.com*

Nanotechnology has been used extensively in the treatment of water and wastewater. The most commonly used techniques for remediation are nano-adsorbents, nano-photocatalysts and nanofiltration membranes. Pharmaceuticals, endocrine-disrupting compounds, cosmetics, dyes etc are recognized as emerging contaminants, whose toxicity is yet to be ascertained. Conventional water treatment techniques have limited efficiency in removing these persistent chemicals. Global efforts to secure clean water continue to be challenged by the increasing detection of emerging pollutants. This work highlights recent advances in nano-remediation, with a particular focus on hybrid strategies that integrate nanoparticle-based adsorbents with cutting-edge nanofiltration technologies. Emphasis is given to nanomaterial fabrication techniques, and surface functionalization techniques which assist precise tuning of physico-chemical characteristics for improved contaminant removal. This work will also focus on re-generation and re-use strategies, ecological safety concerns, and issues related to scaling up fabrication and integrating these technologies into real-world treatment systems. Collectively,

these innovations emphasize the transformative potential of nanotechnology based hybrid approaches for realizing safer, more viable water purification.

### **AEIL-05: High-Valent Iron Species (Fe VI, Fe V, and Fe IV) in Water, Food, Energy, and Health Nexus**

**Virendr K. Sharma**

*Department of Chemical, Environmental, and Materials Engineering,  
University of Miami, Coral Gables 33146, Florida, USA  
E-mail : vks38@miami.edu*

Society is facing numerous challenges like climate change, water scarcity, vector-borne diseases, microbial pathogens, and antibiotics in water. The solution to such difficulties is in innovative approaches that utilize environmentally friendly earth abundant elements having multiple roles. We have been examining the use of high-valent iron oxides as green and advanced molecules in various societal problems. Iron in the plus 6-oxidation state (Ferrate,  $\text{Fe}^{\text{VI}}\text{O}_4^{2-}$ ) has multiple modal actions in oxidizing micropollutants (e.g., antibiotics), in coagulating toxic metals (e.g., arsenic and lead) to achieve water sustainability, and in disinfecting water and surfaces (e.g., *Clostridium difficile* and Murine Norovirus) to enhance population health care. “Activated Ferrate” ( $\text{Fe}^{\text{V}}$  and  $\text{Fe}^{\text{IV}}$ ) are relatively short-lived transients when produced in aqueous solution (e.g.,  $\text{Fe}^{\text{VO}}_4^{3-}$ ,  $\text{Fe}^{\text{IV}}\text{O}_4^{4-}$ ,  $\text{Fe}^{\text{IV}}\text{O}_3^{2-}$ , and  $\text{FeO}^{2+}$ ) and can degrade recalcitrant pollutants and microorganisms in water, and hospital surfaces with high efficiency in seconds, which would otherwise take several minutes or hours by Ferrate without activation. Examples of Ferrate in sterilization of vegetables and fruits and water splitting and recent research on single atom catalysts and metal-organic frameworks in abatement of micropollutants will be presented.

### **AEIL-06: Nanomaterial Modified Sensors for Theranostics: Unveiling a New Horizon in Ultrasensitive Biomedical Detection**

**Sanghamitra Chatterjee**

*Department of Chemistry, Institute of Chemical Technology, Mumbai  
E-mail: sk.chatterjee@ictmumbai.edu.in*

The last few years have witnessed a substantial technological renaissance that boosted the development of nanomaterials which have a great impact on biosensing. The unprecedented properties of carbon nanotubes, fullerenes and graphene have catapulted carbon materials in the hotspot of biomedical research. Of particular interest is the integration of these materials into analytical systems that impact key research areas, in particular: medical diagnostics, multi-modal

drug delivery, bio-imaging, environmental monitoring and biocatalytic sensing. The interface of electrochemistry and nanotechnology is a captivating playground for the elemental research and has eventually emerged as a futuristic and sustainable platform. Efforts have been made in our group to develop new-fangled approaches for the electrochemical detection of non-steroidal anti-inflammatory drug; antihypertensive agent, antiviral drug and natural alkaloid related to hepatocellular carcinoma. The proposed nanomaterial-based sensors exhibited pronounced analytical performance and provided a new and powerful paradigm in terms of novel and augmented functionality that encompasses a wide variety of applications in clinical diagnostics and biological research. The developed electrochemical sensors had great potential for enhancing and superseding the capabilities of current molecular diagnostics by allowing rapid and highly accurate diagnoses, the integration of diagnostic and therapeutic capacities and the realization of personalized medicine.

## **AEIL-07: Advancements in Polymer Electrolyte Fuel Cell Technology: Research Opportunities and Technology Challenges**

**Santoshkumar D. Bhat**

*CSIR-Central Electrochemical Research Institute-Madras Unit,  
CSIR Madras Complex, Chennai  
E-mail: sdbhat.cecri.res.in*

The National Hydrogen Mission has emerged as a pivotal initiative to meet India's surging energy demands and foster the growth of a robust hydrogen ecosystem. Within this context, Polymer Electrolyte Fuel Cells (PEFCs) hold immense promise, particularly in addressing the energy needs of the telecom and automobile sectors and even aviation sectors. This invited talk explores the critical role of PEFCs in the Indian context, focusing on the entire value chain and emphasizing the essential component of the Membrane Electrode Assembly (MEA) where electrochemical reactions occur. The MEA is at the heart of PEFCs, presenting unique material challenges. This presentation delves into the research opportunities within MEA development, highlighting the importance of enhancing ionic conductivity, ensuring membrane electrolyte stability, and exploring alternative catalyst supports. Notably, the talk emphasizes the potential of indigenous membrane electrolyte development as a cost-effective alternative to Nafion® and introduces novel catalyst support materials for enhanced durability in PEFCs, all achievable with simplified and indigenously available processes.

The commercialization of PEFCs faces various technology challenges, including the need to reduce system weight and volume, improve water and thermal management, and lower overall costs. In this context, the talk discusses innovative solutions, such as thin bipolar plates and the adoption of an open cathode fuel cell technology, high temperature fuel cell technology that streamlines system complexities. Collaboration is key to advancing PEFC technology, and this talk highlights ongoing partnerships between academia and industry as a part of CSIR-NMITLI, ANRF, and CSIR-Hydrogen Technology Mission Program. In summary, this invited talk sheds light on the pivotal role of PEFCs within India's National Hydrogen Mission and underscores the significance of research, innovation, and collaborative efforts in advancing PEFC technology to meet the evolving energy needs of the telecom and automobile, drone and other aviation sectors.

### **AEIL-08: Electrochemical Sensors for the Detection of Some Pesticides**

**Nagaraj P. Shetti**

*Centre for Energy and Environment, School of Advanced Sciences, KLE Technological University, BVBCET Campus, Vidyannagar, Hubballi – 580 031, Karnataka*  
*E-mail: npshetti@kletech.ac.in*

Pollution remains a significant challenge due to the ongoing influx of new pollutants into the environment. As a result, there is an urgent need to develop analytical tools that are sensitive, reliable, simple, and selective. Pesticides have been extensively used in agriculture to protect crops from pests; however, their runoff into non-target areas, such as water and soil, leads to environmental contamination. In the field of electroanalytical research, cyclic voltammetry (CV) and square wave voltammetry (SWV) have become widely adopted methods. This analytical study focused on commonly used global pesticides, including carbendazim, pCPA, 2,4-D, diuron, and dichloro. To detect these toxic molecules, carbon and metal-based nanomaterials, along with their composite sensors, were utilized. The developed materials were characterized using various techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), atomic force microscopy (AFM), ultraviolet-visible spectroscopy (UV-Vis), Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), and electrochemical impedance spectroscopy (EIS). These techniques helped evaluate the structural, morphological, and functional aspects of the materials for sensing applications. Sensor validation was achieved

by examining changes in analyte concentration. Optimal conditions for detection were established by assessing the effects of pH, accumulation time, and the quantity of the modifying agent. Additionally, electrokinetic and thermodynamic properties were investigated through studies of scan rate and temperature variations. The developed method successfully monitored pesticide molecules in water and soil samples, highlighting its importance for agricultural and environmental applications.

### **AEO-CYSA-01: Enhanced Non-enzymatic Electrochemical Sensor for 2,6-Diaminopurine based on Nickel phthalocyanine-Modified Carbon Paste Electrode**

**Preemal N. Rodrigues, Vaishnavi Vishwanath and  
Ronald J. Mascarenhas<sup>1\*</sup>**

*Electrochemistry Research Group, Department of Chemistry, St Joseph's  
University, Bangalore, 560027  
E-mail: rodriguesnishma@gmail.com; ronaldmasc@sju.edu.in*

2,6-Diaminopurine (DAP), a purine derivative, is recognized for its potential anticancer and antiviral properties. Despite its therapeutic significance, the pharmacokinetics and potential side effects of DAP remain inadequately characterized, underscoring the necessity for a reliable method to detect trace levels of this compound in pharmaceutical and clinical samples to facilitate precise dosage regulation. In this study, we report the development of a novel electrochemical sensor for DAP detection, achieved through the modification of carbon paste electrodes with nickel phthalocyanine. Electrochemical characterization revealed that DAP undergoes oxidation, exhibiting an anodic peak associated with an irreversible reaction mechanism involving the transfer of two protons and two electrons. The nickel phthalocyanine-modified electrode exhibited enhanced electrochemical performance, characterized by increased surface area and superior responsiveness when compared to unmodified carbon paste electrodes. Its use directly quantified DAP in urine samples, hence suggesting further wide usage in pharmaceutical formulations. Optimizing the experimental conditions showed an excellent linear detection range from  $5.0 \times 10^{-8}$  M to  $1.0 \times 10^{-3}$  M with a detection limit of 1.649 nM and a quantification limit of 5.499 nM. The satisfactory results obtained validate the sensor designed to be effectively applicable for routine monitoring of DAP concentrations in a clinical setting.

## **AEO-CYSA-02 : Polyethyleneimine-Coated Manganese Ferrite Composite: An Efficient and Sustainable Magnetic Adsorbent for Sequestration of Anionic Dye in Aqueous Medium**

**Prachi C. Saraf, Pratik Ghuge and Satish K. Pardeshi\***

*Department of Chemistry, Savitribai Phule Pune University (Formerly University of Pune), Ganeshkhind, Pune, 411007  
Email: satish.pardeshi@unipune.ac.in*

Sunset yellow is a widely used azo dye in the food and pharmaceutical industries due to its vibrant colour; however, due to its chemical stability, it takes longer to degrade in an aqueous environment, causing wastewater pollution. Sunset yellow in wastewater is of concern, as short-term exposure has been associated with allergies and hyperactivity in children, while long-term exposure can cause gastrointestinal issues and potential carcinogenic effects. The adsorption process is a cost-effective and viable method for the removal of azo dyes from wastewater. Herein, polyethyleneimine-coated manganese ferrite (MF-PEI) was fabricated using the hydrothermal method, with the goal of studying its application as a magnetic adsorbent. The successful incorporation of branched-PEI over  $\text{MnFe}_2\text{O}_4$  was studied using XRD, TG-DTA, FT-IR, and XPS analysis. The influence of polyethyleneimine coating on the magnetic properties of manganese ferrite was examined using VSM studies. The effect of various parameters like adsorbent dose, dye concentration, pH, etc, on the adsorption of sunset yellow was investigated using UV-Vis spectroscopy. The maximum dye removal was obtained at pH=4 with 50mg of MF-PEI in 40 minutes, with a maximum adsorption capacity of 12.10 mg/g. The results show that the polyethyleneimine-coated manganese ferrite is an efficient and sustainable magnetic adsorbent for the removal of anionic azo dye like sunset yellow from wastewater.

## **AEO-CYSA-03: Electrochemical Properties of Endocrine-Disrupting Pollutants Bisphenol-A and Tartrazine at $\text{SrAl}_2\text{O}_4$ Modified Carbon Paste Electrode**

**Puneeth and B.E. Kumara Swamy\***

*Dept. of PG Studies and Research in Industrial Chemistry, Kuvempu University, Jnana Sahyadri Shankaraghatta - 577451, Shivamogga (D), Karnataka (S).  
E-mail: bek@kuvempu.ac.in; kumaraswamy21@gmail.com*

Strontium aluminum oxide (SAO) nanoparticles were synthesized using the solution combustion method, with their structure confirmed by XRD, FESEM, and EDS analyses. The study involves developing a



modified electrode enhanced with SAO for detecting bisphenol-A (BPA) and tartrazine (TZ). BPA is incorporated in polycarbonates, epoxy resins, and other plastics to improve toughness, while TZ is a food colorant. However, contamination by BPA and TZ causes endocrine disruption, Alzheimer's disease, and cardiovascular diseases. The electrode demonstrates stability and sensitivity, as demonstrated by cyclic voltammetry (CV) for TZ and BPA. The pH experiments indicate that BPA involves equal sharing of electrons and protons. The scan rate study confirms that both analytes exhibit an adsorption-controlled process. The differential pulse voltammetry (DPV) determines that 0.368  $\mu\text{M}$  and 0.168  $\mu\text{M}$  for BPA and TZ, respectively. The electrode also enables simultaneous detection of uric acid, BPA, and TZ within the same solution. Additionally, real-time testing of BPA and TZ yielded good recovery rates in different samples.

### **AEO-CYSA-04: Selective and Sensitive Detection of Nitrofurantoin via MOF-on-MOF Core-Shell Electrocatalyst**

**Varsha Raj and P. Mallu**

*JSS Science and Technology University, Mysuru-06, Karnataka  
E-mail: varsharaj@jssstuniv.in*

Herein, in this work, we report the fabrication of a novel Cu-BTC@UiO-66 (MOF-on-MOF) core-shell hybrid structure for enhanced electrochemical detection of nitrofurantoin. Nitrofurantoin (NFT), a broad-spectrum urinary antibiotic, is used clinically to treat human bacterial infections are often found in freshwater bodies and marine ecosystems, necessitating the rapid detection and quantification of these drug matrices to ensure health and habitat security. In this work, we have solvothermally synthesized a Cu-BTC@UiO-66 core-shell structure for the electrochemical detection of nitrofurantoin. The structural and morphological characterisations of the as-synthesised material were studied using XRD, FTIR, FESEM, EDX, HRTEM, and BET, which confirmed the successful formation of the Cu-BTC@UiO-66 structure. The electrochemical performance of the developed electrochemical sensor was evaluated by cyclic voltammetry, linear sweep voltammetry, and electrochemical impedance spectroscopy. It is worth noting that the present study achieved a dynamic linear range of 20 $\mu\text{M}$ - 320 $\mu\text{M}$ , a remarkably low Limit of detection (LOD) of 0.381 $\mu\text{M}$ , Limit of quantification (LOQ) of 1.270 $\mu\text{M}$ , and a sensitivity of 6.26  $\mu\text{A}/\mu\text{M}/\text{cm}^2$ . Additionally, Cu-BTC@UiO-66/GCE exhibits outstanding stability, repeatability, and reproducibility. Ultimately, the NFT sensor was successfully implemented in real-time detection and quantifying NFT in tap water and river water samples.



## **AEO-CYSA-05: Green Solvent Extracted Curcumin Incorporated Crosslinked Cellulose-Based Biodegradable Membranes for Food Packaging Application**

**Sachin N. Hegde and Nagraj P. Shetti\***

*Center for Energy and Environment, School of Advanced Sciences, KLE  
Technological University, Hubballi-580031  
E-mail: sachin.hegde@kletech.ac.in; npshetti@kletech.ac.in*

Polymeric materials for food packaging applications have gained significant attention from the research community due to their high demand in the current scenario. In this study, we have synthesized bioactive curcumin employing 50% ethanol as solvent using the Soxhlet apparatus. The green synthesised nano-particles were incorporated into cellulose-formaldehyde crosslinked membranes. The physico-chemical properties of the synthesized curcumin nano-particles and the developed composite crosslinked membranes were characterised using different analytical techniques, including Fourier transform infrared (FT-IR) spectroscopy, UV-Visible spectroscopy, and wide-angle X-ray diffractometry (WAXD). The surface morphology of the developed membranes was studied using a scanning electron microscope (SEM). The moisture uptake, oxidative stability, mechanical stability, antimicrobial activity, and soil degradation studies were employed to check the suitability of the resulting membranes for the food packing application. Among the developed membranes, 2 mass% curcumin incorporated cellulose-formaldehyde crosslinked membrane showed antioxidant capacity value of 51%, and excellent food packaging performance compared to preteen membrane, as well as the commercial polymeric packaging materials, including plastic. This is owing to the presence of curcumin particles. All these results indicate that the developed cellulose-based biodegradable membrane incorporated with green solvent extracted curcumin could be a very good candidate for the food packaging application.

## **AEO-CYSA-06: NiWO<sub>4</sub>/reduced graphene oxide modified electrode for ultra-sensitive nanomolar detection of Cu(II) and Hg(II) in environmental samples**

**Raveendra B. Manami and Rajesh G. Kalkhambkar\***

*Department of Chemistry, Karnatak University's Karnatak Science College,  
Dharwad, Karnataka 580001  
E-mail: raveendram57@gmail.com*

Heavy metals like Cu(II) & Hg(II) are poisonous, persistent may

accumulate in living things, making their detection essential. They provide significant dangers to human health & the environment, even at low concentrations. Pollution control, public safety & environmental monitoring all depend on sensitive & trustworthy detection techniques. A  $\text{NiWO}_4/\text{RGO}$  nanocomposite has been produced utilizing a simple reflux method by integrating nickel tungsten oxide ( $\text{NiWO}_4$ ) nanoparticles with reduced graphene oxide. This composite was applied for modifying a glassy carbon electrode, resulting in a  $\text{NiWO}_4/\text{RGO}/\text{GCE}$  sensor capable of simultaneously detecting  $\text{Cu(II)}$  &  $\text{Hg(II)}$  ions in environmental samples. Characterization techniques as SEM, EDS, FTIR, PXRD & Raman spectroscopy confirmed the successful formation of the nanocomposite. Electrochemical studies using CV & DPASV demonstrated high sensitivity, selectivity & reproducibility. The sensor showed an enormous linear range (1–20 ppb) & extremely low detection limits: 0.142 ppb for  $\text{Cu(II)}$  & 0.120 ppb for  $\text{Hg(II)}$ . Real sample analysis showed excellent recovery rates ranging from 97.8 to 102.0%, indicating strong practical applicability. This work presents a cost-effective & reliable electrochemical platform for trace heavy metal detection, with promising potential for environmental monitoring applications.

## **AEO-CYSA-07: Transforming Polyethylene Terephthalate into Dyes for Optoelectronic Applications**

**Neha Mittal\* and R.K. Soni**

*Department of Chemistry, Chaudhary Charan Singh University, Meerut, U.P.  
E-mail : mittaln671@gmail.com*

The escalating production of polyethylene terephthalate (PET) waste poses a critical environmental threat, calling for innovative and sustainable upcycling strategies. This study presents an eco-conscious approach to transforming PET waste into functional bis-azo dyes with promising applications. Post-consumer PET bottles were chemically aminolyzed using para-phenylenediamine, followed by diazotization and coupling with phenolic derivatives to synthesize structurally tailored bis-azo dyes. These dyes were thoroughly characterized through UV-Visible spectroscopy, FTIR, Thin Layer Chromatography, and other analytical techniques. The synthesized compounds demonstrated strong absorption in both UV and visible regions, suggesting their potential utility in optoelectronic devices such as dye-sensitized solar cells (DSSCs). This research not only provides a route for waste valorization but also contributes to the development of dye materials that support cleaner energy technologies and ecological preservation.

## **AEO-CYSA-08: AI-Assisted Synthesis of Alkyl Polyglucoside Sulfate-Based Tin(IV) Phosphate: A Novel Cation Exchanger for Environmental Applications, Particularly Water Purification**

**Amita Somya<sup>1\*</sup> and Amit Prakash Varshney<sup>2</sup>**

<sup>1</sup>*Department of Chemistry, Amity School of Applied Sciences, Amity, University, Bengaluru-562110, Karnataka*

<sup>2</sup>*Independent Researcher, Begaluru-560064, Karnataka*

*E-mail: asomya@blr.amity.edu*

Alkyl polyglucoside sulfates (APGS) are promising eco-friendly anionic surfactants due to their excellent surface activity, biodegradability, and renewable origin. In this study, a novel composite cation exchanger based on APGS-modified tin(IV) phosphate (APGS-SnP) was synthesized and characterized for environmental applications, particularly water purification. Incorporation of APGS into the tin(IV) phosphate matrix enhanced surface functionality, dispersibility, and structural stability. FTIR, XRD, and SEM analyses confirmed successful anchoring of APGS molecules, improving porosity and active site availability. The composite exhibited higher ion-exchange capacity and better adsorption of Cd(II) and Cu(II) ions than pristine tin(IV) phosphate. Artificial Intelligence (AI) tools were employed to optimize synthesis and evaluate performance. Machine learning models trained on experimental data predicted ion-exchange capacity and adsorption efficiency under varying conditions, enabling rapid identification of key parameters. AI-guided optimization supported the selection of favorable synthesis and operational conditions for enhanced contaminant removal. This integration of renewable surfactant chemistry, inorganic ion-exchangers, and AI provides a sustainable and data-driven strategy for developing multifunctional materials for efficient water treatment and environmental remediation.

## **AEO-CYSA-09: Micro- and Nano-Plastics in Urban Air: Polymer Composition, Interactions and Inhalation Risk**

**Ankush Kaushik<sup>1</sup>, Anju Elizbath Peter<sup>1</sup>, Manuela van Pinxteren<sup>1</sup>, Barbara M. Scholz-Böttcher<sup>2</sup> and Hartmut Herrmann<sup>1\*</sup>**

<sup>1</sup>*Atmospheric Chemistry Department (ACD), Leibniz Institute for Tropospheric Research (TROPOS), Permoserstraße 15, Leipzig, 04318, Germany*

<sup>2</sup>*Institute for Chemistry and Biology of the Marine Environment (ICBM), Carl von Ossietzky University of Oldenburg, P.O. Box 5634, D-26046 Oldenburg, Germany*

*E-mail: kaushik@tropos.de*

Airborne micro- and nano-plastics are an emerging yet overlooked component of urban air pollution, having direct implications on human

health. This study quantified their concentrations and polymer composition in size-fractionated particulate matter collected in Leipzig, Germany, using pyrolysis-gas chromatography-mass spectrometry. The total mass of plastic particles smaller than 10  $\mu\text{m}$  averaged  $0.6 \pm 0.2 \mu\text{g}/\text{m}^3$ , with fine and coarse fractions contributing almost equally. Tire-wear particles dominated (60-65%) the polymer distribution, accounting for roughly two-thirds of the measured plastic mass, followed by polyethylene (12-17%), polyvinyl chloride (12-14%), and polyethylene terephthalate (4-7%). Strong correlations exist between quantified polymers and carbonaceous aerosols, reflecting their shared sources of emission and atmospheric mixing processes. Estimated inhalation exposure suggests that adults may inhale approximately 2.1  $\mu\text{g}$  of airborne plastic particles per day. Using established particulate-matter risk models, this level of exposure is linked to roughly a 9% rise in cardiopulmonary mortality and 13% rise in lung-cancer mortality compared with baseline conditions. By combining polymer-specific measurements with exposure and health-risk analysis, this study demonstrates that inhalable micro- and nano-plastics form a meaningful fraction of urban particulate pollution and highlights the need for targeted regulatory measures and region-specific data to inform air-quality and public-health policy.

## **AEO-CYSA-10: Electrocatalytic Detection and Photocatalytic Degradation of 4-Aminophenol using $\text{Cu}_2\text{O}/\text{BiOCl}$ Nano-Heterojunction**

**Sobandhar Prakash Bharath Kumar and Ningappa Kumara Swamy\***

*Department of Chemistry, JSS Science and Technology University, Mysuru-570006, Karnataka*

*E-mail: bharathkumarsp2381999@gmail.com; kumaryagati@gmail.com*

A Copper oxide/Bismuth oxychloride ( $\text{Cu}$ ,  $\text{O}/\text{BiOCl}$ ) heterojunction was synthesized using a low-temperature liquid-phase method and used for the electrochemical detection and photocatalytic degradation of 4-aminophenol (4-AP). The material was characterized by using spectroscopic and microscopic techniques. For electrochemical detection, a Glassy carbon electrode (GCE) was modified with  $\text{Cu}$ ,  $\text{O}/\text{BiOCl}$  nano-heterojunction and a GCE/ $\text{Cu}$ ,  $\text{O}/\text{BiOCl}$  sensor was constructed. The constructed GCE/ $\text{Cu}$ ,  $\text{O}/\text{BiOCl}$  sensor showed well-defined redox peaks. Cyclic voltammetry (CV) and linear sweep voltammetry (LSV) studies on the constructed sensor showed a sensitive response, with a limit of detection (LOD) of 0.165  $\mu\text{M}$ , a limit of quantification (LOQ) of 0.555  $\mu\text{M}$ , a sensitivity of 1.765  $\mu\text{A}/\mu\text{M cm}^2$ , a linear range of 1-20  $\mu\text{M}$  and high selectivity. The real sample analysis showed an excellent recovery rate, assuring the GCE/ $\text{Cu}$ ,  $\text{O}/$

BiOCl sensor for reliable detection and quantification of 4-AP in pharmaceutical samples. Additionally, the Cu, O/BiOCl nano-heterojunction was employed as an efficient photocatalyst for 4-AP degradation under visible light (9 W LED). The photocatalytic efficiency was 98.2% at an optimal catalyst dose of 10 mg and degradation was found to follow pseudo-first-order kinetics. Radical trapping experiments indicated that  $\bullet\text{OH}$  and  $\text{h}\nu$  were the dominant reactive species in the degradation process. Stability and reusability tests confirmed the catalyst's durability. Further, the phytotoxicity studies were conducted on treated solution using mung bean and cowpea seeds, which showed enhanced germination and seed growth, suggesting the suitability of treated water in agriculture. Antibacterial studies against *S. aureus* and *E. coli* further supported its environmental safety. Overall, the Cu, O/BiOCl heterojunction has the potential to serve as a bifunctional material for both electrochemical detection and photocatalytic removal of 4-AP.

### **AEO-CYSA-11: Artificial Intelligence Enhancing Efficiency, Safety, and Sustainability in Chemical Engineering**

**Ashok G. Matani**

*Department of Mechanical Engineering, Government College of Engineering, Jalgaon 425001 (M.S.)*

*E-mail: dragmatani@gmail.com, ashokgm333@rediffmail.com*

Artificial Intelligence (AI) is a powerful tool for reducing safety and hazmat risks in chemical transportation. The benefits of predictive maintenance, route optimization, driver behavior monitoring, hazard detection, and emergency response optimization make AI an invaluable asset for managing hazmat operations. By leveraging AI, chemical engineers are now able to unravel complex chemical processes, predict outcomes with greater accuracy, and streamline operations in ways previously unimaginable.

### **AEO-CYSA-12: Enhanced Photoelectrochemical and Photocatalytic Water Splitting by Indium-Doped CdS@ZnO Heterostructures Grown on FTO via SILAR Method**

**Swapnil R. Lande and Satish K. Pardeshi\***

*Department of Chemistry, Savitribai Phule Pune University (formerly University of Pune), Ganeshkhind, Pune, 411007*

*E-mail : satish.pardeshi@unipune.ac.in*

Indium-doped CdS@ZnO (In-CdS@ZnO) heterostructures with 1–4% In were successfully grown on FTO substrates by the successive

ionic layer adsorption and reaction (SILAR) method. XRD and SAED confirmed the crystalline CdS@ZnO heterojunction, while XPS verified In<sup>3+</sup> incorporation into both CdS and ZnO lattices. HR-TEM images showed uniform nanostructures with an average particle size of 21.8 nm. UV–visible spectra revealed extended visible-light absorption and a narrowed band gap of 2.33 eV for the optimized 3% In–CdS@ZnO sample. PL analysis indicated a reduction in the recombination of photogenerated carriers. The optimized photoelectrode exhibited a photocurrent density of 2.31 mA cm<sup>-1</sup> vs. Ag/AgCl, nearly six times higher than that of ZnO, and achieved a photocatalytic hydrogen evolution rate of 1519.9  $\mu\text{mol/g/h}$  under visible light. These results demonstrate that controlled doping and SILAR-based growth significantly enhance charge transfer and light harvesting, making 3% In–CdS@ZnO a promising photocatalyst for efficient PEC water splitting.

### **AEO-CYSA-13: Synergistic Photocatalytic Performance of a CoMgLDH/Ni-Borophene Composite for Hydrogen Evolution and Dye Degradation**

**Madasu Sreenivasulu and Nagaraj P. Shetti\***

*Center for Energy and Environment, School of Advanced Sciences,  
KLE Technological University, Hubballi-580031, Karnataka  
E-mail: m.sreenivasulu@kletech.ac.in; npshetti@kletech.ac.in*

A key challenge in particulate photocatalytic water splitting is the rapid recombination of photogenerated charge carriers, which significantly limits the efficiency of the HER. Although Z-scheme systems provide partial mitigation, they often encounter issues related to shuttle ion adsorption. In this work, we report a novel CoMgLDH/Ni-Borophene (Ni-BPN) composite photocatalyst, synthesized via a facile hydrothermal method and designed to improve intrinsic efficiency through a tailored Type-II heterojunction. Spectroscopic and electrochemical analyses confirm that metallic Ni-BPN functions as an effective electron sink, facilitating directional electron transfer from the conduction band of CoMgLDH to Ni-BPN, while retaining holes on the LDH. This mechanism effectively suppresses electron-hole recombination. The CoMgLDH/Ni-BPN composite demonstrates excellent HER performance, achieving a hydrogen evolution rate of 22.43  $\text{mmol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$  under visible light, 2.2 times higher than pure CoMgLDH (10.23  $\text{mmol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ ) and 2.4 times that of Ni-BPN alone (9.52  $\text{mmol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ ). Additionally, the composite exhibits remarkable stability over prolonged illumination and repeated cycles. The enhanced activity arises from the synergistic combination of CoMgLDH's high



surface area and strong visible-light absorption with Ni-BPN's superior charge separation and conductivity. This study presents a promising strategy for designing efficient, stable metal-conductor-based heterojunction photocatalysts, advancing mediator-free heterogeneous

### **AEO-CYSA-14: Electrochemical Sensing of An Anticancer Drug Temozolomide using Carbon Paste Electrode Enriched with Porous Carbon Nanotubes and Highly Conductive Titanium Carbide**

**P.R. Kulkarni<sup>1</sup> and J.C. Abbar<sup>2</sup>**

<sup>1</sup>*Department of Chemistry, BLDEA'S, S.B. Arts and K.C.P. Science College, New Campus Vijayapur-586103*

<sup>2</sup>*BMS Institute of Technology and Management, Bengaluru 560119*  
*E-mail: vaishnavikulkarni140@gmail.com*

Due to an increased rate of mortality associated with the tumoral disease, the demand has driven pharmaceutical industries to focus on synthesizing the chemotherapeutic drug in precise concentrations and compositions to fulfil the needs and aid in disease treatment. Likewise, temozolomide (TMZ), an antitumor drug, has gained significant importance, and so its determination is very essential. The multi-walled carbon nanotubes and titanium carbide nanoparticles were used to prepare the carbon paste-modified sensor for the investigation of TMZ using voltametric, surface and electrochemical impedance spectroscopy (EIS) techniques. The surface properties were analysed using SEM and EDX. The cyclic voltammetry studies showed that TMZ detection in a 0.2M phosphate buffer solution gave two oxidation peaks and a reduction peak. Using the differential pulse voltametric method, the limit of detection (LOD) was calculated within the linear range of 0.3V to 1.1V as  $1.64 \times 10^{-7} \text{M}$  and  $5.2 \times 10^{-8} \text{M}$  for both oxidation peaks. Analytical electrochemical functions have been cleared by the reported sensor for the detection of TMZ in pharmaceutical formulations and real samples like human plasma, urine and water samples.

### **AEO-CYSA-15: Ion-Exchange Behavior of Admicellar CTAB Layers on Glassy Carbon Electrode Revealed by Ferricyanide-Mediated Ascorbic Acid Oxidation**

**Kumar Sandhya<sup>1,2</sup> and Annamalai Senthil Kumar<sup>\*1,2</sup>**

<sup>1</sup>*Nano and Bioelectrochemistry Research Laboratory, Carbon dioxide Research and Green Technology Centre, Vellore Institute of Technology University, Vellore-632 014*

<sup>2</sup>*Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology University, Vellore-632 014*  
*E-mail : askumar@vit.ac.in; askumarchem@yahoo.com*

The structure and molecular dynamics of surfactant-driven

assemblies at the electrode-electrolyte interface remain an active area of research, particularly for mimicking biomembrane like systems and developing novel application platforms. The structural and dynamic characteristics of these assemblies are strongly influenced by both solution-phase and electrode-surface parameters. In this study, a thin layer of the cationic surfactant cetyltrimethylammonium bromide (CTAB) was adsorbed on a glassy carbon electrode (GCE) using an ethanol-assisted modification process. This modification yielded highly ion-exchangeable organized assemblies, which were investigated using ferricyanide ions as a probe via cyclic voltammetry in an aqueous medium. Physicochemical, electrochemical, and scanning electrochemical microscopy (SECM) analyses revealed that CTAB adsorption under electrified conditions on GCE leads to the formation of adlayer and admicelles -like multilayered organized assemblies. These structures are stabilized by non-Coulombic interactions between the hydrophobic domains of the CTAB aggregates and the hydrophobic basal planes of the GCE, facilitating subsequent electron-transfer reactions. As a practical demonstration, in situ formation of Prussian Blue (PB) was achieved using the {CTAB}-  $\text{Fe}(\text{CN})_6^{3-}$  assembly as a template in the presence of  $\text{Fe}^{2+}$  ions. Furthermore, the modified surface, {CTAB}-  $\text{Fe}(\text{CN})_6^{3-}$  enabled selective and sensitive heterogeneous mediated oxidation of ascorbic acid via the confined ferricyanide/ferrocyanide redox couple. Overall, the findings of this study provide a new perspective on surfactant-adlayer-modified electrode surfaces, highlighting their potential for real-time electrochemical applications.

### **AEO-CYSA-16: Methionine polymerized Chitosan Composite Sensor for the Sensitive Detection of Azithromycin**

**K.P. Moulya and J.G. Manjunatha\***

*Department of Chemistry, FMKMC College, Constituent College of Mangalore university, Karnataka  
E-mail: manju1853@gmail.com*

The present study aimed to design an electrochemical sensor for the analysis of azithromycin (AZ) by modifying the bare chitosan composite paste electrode (BCPE) surface using methionine (MT) in 0.2 M of phosphate buffer solution (PBS). Cyclic voltammetry (CV) was employed for fabricating poly methionine modified chitosan composite paste electrode (PMT/CSCPE) and the surface morphology was studied by applying electrochemical impedance spectroscopy (EIS) and linear sweep voltammetry (LSV). Various parameters such as pH, scan rate, accumulation time and potential were employed to evaluate



the efficiency of the developed electrode to detect AZ. The impact of AZ concentration variation on the oxidation peak current was assessed using CV and LSV in the linear range of 2.0 to 80.0  $\mu\text{M}$  with the limit of detection (LOD) of 0.621  $\mu\text{M}$  and 0.335  $\mu\text{M}$  respectively. Moreover, PMT/CSCPE demonstrates excellent sensitivity and selectivity in detecting AZ, even in the presence of other interferents. The PMT/CSCPE was effectively used for the analysis of real samples.

## **AEO-CYSA-17: Integrated Electrochemical Biosensing Platform for Portable and Multiplex AMR Diagnostics**

**Madaje Amir Ibrahim<sup>1,2</sup>, Shinde Pritam Venkatrao<sup>1,2</sup>, Sonal Fande<sup>1,3</sup>, D. Sriram<sup>3</sup> and Sanket Goel<sup>1,4</sup>**

<sup>1</sup>*MEMS, Microfluidics and Nanoelectronics Lab, Department of Electrical and Electronics Engineering, Birla Institute of Technology and Science, Hyderabad, 500078*

<sup>2</sup>*Department of School of Interdisciplinary Research and Entrepreneurship (SIRE), Birla Institute of Technology and Science, Hyderabad, 500078*

<sup>3</sup>*Department of Pharmacy, Birla Institute of Technology and Science, Hyderabad, 500078*

<sup>4</sup>*Department of Electrical and Electronics Engineering, Birla Institute of Technology and Science, Hyderabad, 500078*  
E-mail : sgoel@hyderabad.bits-pilani.ac.in

Antimicrobial resistance (AMR) has emerged as a critical global health challenge, undermining the effectiveness of existing antibiotics and leading to increased morbidity, mortality, and healthcare costs. It requires rapid diagnostic approaches, as conventional antimicrobial susceptibility testing (AST) typically requires 24–48 hours to produce actionable results. This study presents a compact electrochemical platform that enables rapid AST and minimum inhibitory concentration (MIC) determination within 4–6 hours using cyclic voltammetry (CV). The device incorporates eight sample wells for simultaneous analysis of eight antibiotics, each with seven concentration levels, facilitating efficient MIC profiling. A temperature-controlled incubation unit (37 °C) and voltage-regulated environment ensure stable bacterial growth conditions before electrochemical interrogation. CV measurements, performed using a laboratory Potentiostat, capture changes in redox behaviour corresponding to bacterial metabolic activity under antibiotic exposure. Future development aims to integrate an IoT-enabled miniaturized Potentiostat, making the platform fully portable and suitable for point-of-care application. This electrochemical approach offers a rapid, multiplex, and scalable solution for AMR detection, significantly reducing diagnostic time and supporting timely therapeutic intervention.

## **AEO-CYSA-18: Vitamin B<sub>12</sub>-Decorated MWCNTs as Enzyme-Mimetic Electrocatalysts Achieving ~100% Faradaic Efficiency in CO<sub>2</sub> Reduction Reaction**

**Yashly Yesudas K.<sup>1,2</sup>, Buvaneswari Gopal<sup>2\*</sup> and Annamalai Senthil Kumar<sup>1,2\*</sup>**

<sup>1</sup>Carbon Dioxide Research and Green Technology Centre, Vellore Institute of Technology University, Vellore 632 014

<sup>2</sup>Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology University, Vellore 632 014

E-mail : askumar@vit.ac.in; askumarchem@yahoo.com

With global CO<sub>2</sub> emissions steadily rising due to rapid industrialisation and heavy reliance on fossil fuels, the development of efficient and selective CO<sub>2</sub> conversion technologies has become increasingly critical. Electrochemical CO<sub>2</sub> reduction (CO<sub>2</sub>RR) is particularly attractive because it operates under mild conditions, requires minimal catalyst loading, and can be tuned to produce specific value-added products. Inspired by the natural enzyme Carbon Monoxide Dehydrogenase (CODH), where a metal centre is precisely positioned and stabilised by a protective protein environment, we adopt a biomimetic strategy to improve catalytic efficiency. In this approach, Vitamin B12, a cobalt-corrin complex known for its redox versatility, is anchored onto a multi-walled carbon nanotube (MWCNT) scaffold. The resulting MWCNT@B12 hybrid catalyst combines the molecular specificity of B12 with the high conductivity and large surface area of carbon nanotubes, offering a stable and efficient platform for CO<sub>2</sub> reduction. The resulting MWCNT@B12 electrode displays a clear surface-confined redox response at E° = -0.72 V vs. Ag/AgCl, confirming effective surface immobilization. Under CO<sub>2</sub>-saturated conditions, the catalyst delivers excellent performance, achieving nearly 100% Faradaic efficiency, a low overpotential of 242 mV, and a current density of 43.5 mA cm<sup>-2</sup> for CO production in 0.5 M NaHCO<sub>3</sub> solution. These findings demonstrate the promise of Vitamin B12-based biomimetic systems for future sustainable CO<sub>2</sub> conversion technologies.

## **AEO-01: Spectrophotometric Estimation of Fluoride Using Marigold Flower Extract: A Green Approach**

**Kashika Tiwari and Priyanka Jain\***

IIS (deemed to be University), Jaipur, Rajasthan

E-mail: priyanka.chemistry@iisuniv.ac.in

A novel, environmentally friendly spectrophotometric method for fluoride determination has been developed using marigold (*Tagetes erecta*) flower extract as a natural chromogenic reagent. The method is based on the competitive binding between fluoride ions and

flavonoids present in marigold extract for aluminum(III) ions, resulting in a measurable decrease in absorbance at 415 nm. Optimal analytical conditions were established through comprehensive optimization studies, including pH 4.95, 10-minute reaction time at room temperature, and specific reagent concentrations. The method demonstrated excellent analytical performance with Beer's law adherence in the range of 1-50 ppm, molar absorptivity of  $3.6 \times 10^2 \text{ L mol}^{-1} \text{ cm}^{-1}$ , detection limit of  $1.024 \text{ } \mu\text{g mL}^{-1}$ , and quantitation limit of  $3.103 \text{ } \mu\text{g mL}^{-1}$ . Recovery studies confirmed the method's accuracy and precision, particularly in the lower concentration ranges. This green analytical approach eliminates the use of toxic organic solvents and hazardous chemicals while maintaining analytical reliability comparable to conventional methods, making it suitable for routine environmental monitoring and water quality assessment.

## **AEO-02: Valorization of Agricultural Waste into High-Performance Cellulose-PES Membranes for Advanced Wastewater Remediation: A Sustainable Approach**

**D.S. Aditya<sup>1</sup>, A.B. Hemavathi<sup>2</sup>, D. Kalpana<sup>3</sup>, G. Gnanakumar<sup>4</sup> and S.K. Nataraj<sup>1\*</sup>**

<sup>1</sup>Centre for Nano & Material Sciences, JAIN University, Jain Global Campus, Bangalore- 562112

<sup>2</sup>Department of Polymer Science and Technology, Sri Jayachamarajendra College of Engineering, JSS Science and Technology University, Mysore-570006

<sup>3</sup>CSIR-Central Electrochemical Research Institute – Madras Unit, CSIR-Madras Complex, Chennai, 600113, Tamil Nadu

<sup>4</sup>Department of Chemistry, Madurai Kamaraj, Palkalai Nagar, Madurai, Tamil Nadu 625021

E-mail: sk.nataraj@jainuniversity.ac.in; sknata@gmail.com

A sustainable strategy was developed to upcycle agricultural biowaste into high-performance cellulose membranes using green extraction methods, thereby eliminating the need for toxic ionic liquids. The extracted cellulose was incorporated into polyethersulfone (PES) to fabricate mixed matrix membranes (C-PS-4), demonstrating the potential of renewable resource utilization in advanced membrane technologies. The resulting membranes exhibited excellent structural stability, superior flux ( $1021 \text{ L.m}^{-2}.\text{h}^{-1}$ ), and strong solute rejection. They also showed broad selectivity by efficiently removing salts together with cationic, anionic, and neutral dyes, while anti-fouling studies confirmed excellent fouling resistance and consistent flux recovery in long-term runs using simulated wastewater (SWW). To validate real-world applicability, the membranes were challenged with hazardous industrial wastewater treatment scenarios, including

tannery and molasses effluents, achieving high flux and rejection even under harsh operating conditions. Extended continuous operation for 200 h with the same industrial effluents further demonstrated the membranes' robustness, stability, and high membrane durability, while consistently maintaining strong performance. Beyond technical efficiency, this approach provides an environmentally benign alternative that transforms agricultural residues into advanced functional materials. This valorization pathway supports circular economy principles by reducing waste streams, conserving resources, and minimizing environmental impact. Overall, the study establishes biowaste-derived cellulose membranes as a scalable and eco-friendly platform for advanced wastewater purification, effectively integrating sustainability with industrial applicability in water management.

### **AEO-03: Advanced RP-HPLC-UV Method for Analyzing PET Waste-Derived Terephthalamides: Method Optimization & Validation**

**Shifa Altaf<sup>1\*</sup>, Rakesh Kumar Soni<sup>1</sup> and Rahul Singhal<sup>2</sup>**

<sup>1</sup>*Department of Chemistry, Chaudhary Charan Singh University, Meerut, 250004, (U.P)*

<sup>2</sup>*Department of Physics & Engineering Physics, Central Connecticut State University, New Britain, CT 06050, USA*

*E-mail : shifa0530@gmail.com*

Polyethylene terephthalate (PET) waste has become a major global environmental concern due to its high production volume and limited biodegradability. Chemical depolymerization offers a promising route for converting PET into valuable intermediates such as N,N'-disubstituted terephthalamides, which can serve as precursors for specialty chemicals and polymers. In this work, a reliable RP-HPLC-UV method was developed for the qualitative and quantitative analysis of these terephthalamide derivatives obtained from PET depolymerization. Key analytical parameters, including linearity, precision, accuracy, limit of detection, and limit of quantification, were evaluated to ensure method suitability for routine laboratory and industrial monitoring. Chromatographic performance indicators such as theoretical plates, resolution, retention behavior, and peak symmetry demonstrated strong separation quality under optimized conditions. The method also aligns with the principles of environmental and analytical sustainability by supporting chemical recycling initiatives and enabling effective valorization of plastic waste. A workflow for application to real PET waste streams is proposed, highlighting the role of chromatography in sustainable materials management. This study demonstrates an efficient analytical platform for tracking PET depolymerization products, contributing to analytical method

development and environmental monitoring in polymer recycling research.

### **AEO-04: Thermal Analysis of Pure and Turmeric-Doped Mustard Oil with Kinetic Approximations of their Oxidation steps**

**Anit Kumar<sup>1</sup> and R.K. Verma<sup>2</sup>**

*<sup>1</sup>Department of Chemistry, C. M. Science College, Darbhanga (LNMU), Bihar*

*<sup>2</sup>University Department of Chemistry, Magadh University, Bodh Gaya, Bihar*

*E-mail : anitchemika@gmail.com; profrkverma@gmail.com*

This study investigates the effectiveness of turmeric as a natural antioxidant in enhancing the thermo-oxidative stability of mustard oil. Differential Scanning Calorimetry (DSC) was employed to analyze thermal behavior at multiple heating rates. Kinetic parameters, including activation energy ( $E_a$ ) and pre-exponential factor ( $A$ ), were calculated using the model-based Kissinger method and the model-free Ozawa–Flynn–Wall (OFW) method. The addition of turmeric led to a significant increase in  $E_a$ , indicating enhanced thermal resistance and delayed degradation of the oil. Furthermore, oxidative stability was assessed using the Peter Simon Induction Period Method, which measures oxidative induction time (OIT). Turmeric doped sample exhibited longer induction periods compared to untreated mustard oil, confirming enhanced resistance to oxidation. These combined findings demonstrate that turmeric effectively improves both the thermal and oxidative stability of mustard oil, highlighting its potential as a natural, safe, and cost-effective antioxidant for edible oil preservation. This work supports the broader application of plant-based additives in enhancing the shelf life and quality of food-grade oils.

### **AEO-05: HPLC-MS/MS Characterized Metabolites of Valeriana wallichii Target BRAF/MEK Signaling in Melanoma**

**Charushila Balikai<sup>1,2\*</sup>**

*<sup>1</sup>PG Department of Chemistry, SKE Society's Govindram Seksaria Science College(Autonomous), Belagavi-590006*

*<sup>2</sup>Department of Chemistry, Centre for Nanoscience and Nanotechnology, KLS G ogte Institute of Technology (Autonomous), affiliated to Visvesvaraya Technological University, Belagavi, Karnataka*

*E-mail: charu@gssbgm.edu.in*

Valeriana wallichii (mâ lù róng cào), a traditional medicinal herb, is recognized for its pharmacological potential. This study investigates its anticancer activity against A375 human melanoma cells using an integrated in silico and in vitro approach. Ultrasonication-assisted hydroalcoholic extraction followed by HPLC-MS/MS profiling identified

chlorogenic acid and quinic acid as major constituents. Network pharmacology linked these metabolites to melanoma-related pathways, particularly MAPK, PI3K-Akt, and Ras, with emphasis on BRAF and MEK nodes. Molecular docking revealed strong interactions of chlorogenic acid at ATP-binding domains of BRAF (CYS532, ASP594, LYS483, GLY534) and MEK (SER150, ALA95), showing affinities comparable to dabrafenib and DS03090629. Molecular dynamics simulations (100 ns) confirmed complex stability, while ADME analysis indicated favorable drug-like properties. In vitro cytotoxicity assays demonstrated significant growth inhibition of A375 cells ( $IC_{50} = 172.8 \pm 1.07 \mu\text{g/mL}$ ), and scanning electron microscopy revealed enhanced cell membrane disruption, likely due to improved bioactive extraction efficiency.

Overall, these findings highlight chlorogenic acid as a promising dual BRAF/MEK inhibitor and validate the traditional use of *V. wallichii* as a potential source of multitargeted therapeutics for melanocytic carcinoma.

## **AEO-06: Application of Waste Cooking Oil As A Biofuel**

**N.C Kothiyal<sup>1</sup> and Sakshi Bawa<sup>2</sup>**

<sup>1,2</sup>*Department of Chemistry, Dr B R Ambedkar National Institute of Technology, Jalandhar, 144011, Punjab*  
E-mail: kothiyalnc@nitj.ac.in

The increasing global energy demand, coupled with severe environmental concerns over the combustion of fossil fuels, necessitates the development of sustainable and renewable alternative energy sources. Waste Cooking Oil (WCO) presents a significant environmental disposal challenge, yet simultaneously offers a highly viable and cost-effective feedstock for producing biodiesel. This study examines the application of WCO as a renewable biofuel through the transesterification process. The WCO was filtered and chemically processed using a catalyst (e.g., potassium hydroxide) and an alcohol (e.g., methanol) to convert triglycerides into fatty acid methyl esters (FAMEs), the primary component of biodiesel. The resulting biofuel was characterised using ASTM standards, confirming its compatibility with conventional diesel engines, particularly in terms of kinematic viscosity, flash point, and cetane number. The use of WCO-derived biodiesel offers substantial environmental benefits, including a significant reduction in net greenhouse gas emissions compared to petroleum diesel, and provides a sustainable solution for waste management. The findings confirm that WCO is an effective and environmentally sound alternative resource capable of mitigating both



waste disposal issues and reliance on finite fossil fuels, thereby supporting the transition to a circular economy and a cleaner energy matrix.

### **AEO-07: Electrochemical analysis of Sulfamethoxazole by CuFe<sub>2</sub>O<sub>4</sub>@f-CNF composite nanoparticle using carbon paste electrode**

**H.R. Dhruthi and B.E. Kumara Swamy\***

*Dept. of PG Studies and Research in Industrial Chemistry, Kuvempu University, Jnana Sahyadri Shankaraghatta - 577451, Shivamogga (D), Karnataka (S).*

*E-mail : kumaraswamy21@gmail.com; bek@kuvempu.ac.in*

The environmental pollutant drug sulfamethoxazole was evolved by carbon paste electrode altered with CuFe<sub>2</sub>O<sub>4</sub>@f-CNF nanocomposites. CuFe<sub>2</sub>O<sub>4</sub> was synthesized by reflux approach and characterized by X-ray Diffraction (XRD), Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), and Fourier Transform Infrared Spectroscopy (FT-IR) techniques. Cyclic voltammetry, Electrochemical Impedance Spectroscopy (EIS), Differential Pulse Voltammetry (DPV), techniques were enforced and the prepared nanocomposite exhibit good conductivity, and large surface area to detect the electrochemical oxidation of sulfamethoxazole. In the optimal condition, compared to a bare carbon paste electrode, the CuFe<sub>2</sub>O<sub>4</sub>@f-CNF modified carbon paste electrode shows good peak current. In addition, the modified electrode evidence good stability, selectivity, repeatability and reproducibility. The modified electrode is also tested and got a satisfactory recovery result for real samples like tap and pond water. Thus, the CuFe<sub>2</sub>O<sub>4</sub>@f-CNF/CPE sensor has promising applications in environmental protection.

### **AEO-8: Reverse Phase-HPLC Method for the Estimation of Doxorubicin in Bulk and Pharmaceutical Dosage Forms**

**Mahesh R.T. and Arunkumar M. Shirahatti**

*Department of Chemistry J.S.S. Banashankari Arts, Commerce & S.K. Gubbi Science College, Vidyagiri, Dharwad - 580 004 (Karnataka)*  
*E-mail: drrtmahesh@gmail.com*

The current research goal was to develop a novel specific method for the quantitation of the Doxorubicin. The method development was done by using a High-Performance Liquid Chromatography (HPLC). The extensive method development was conducted to identify a right combination of chromatographic conditions and validated as per the regulatory guidelines. The simple combination of organic modifier

and buffer (40:60) used to elute the Doxorubicin in isocratic mode. The shorter run time of the method was achieved by optimizing the flow rate of 0.8mL per minute along with L1-octadecyl chemistry column. The doxorubicin peak was detected by using a sensitive Ultra violet detector at 254nm. The purity threshold of more than 990 proves that the method is free from any possible interferences and the linearity was established at 5 different levels with a correlation coefficient 0.999. The overall %RSD (relative standard deviation) of mean recovery was 1.1%. The marketed commercial formulation of Doxorubicin injection was tested on the developed method to confirm the suitability of the method for both bulk active substance and pharmaceutical formulations. Based on the experimental outcome method can be regarded as inventive, short run time, specific to quantitate Doxorubicin.

### **AEO-9: Efficacious Surface Engineering of a Carbon Paste Electrode for Detecting the Myorelaxant Antispasmodic Drug using Nanostructured Zirconium Oxide Enhanced with Cetyltrimethylammonium Bromide: Insights into Electrochemical Sensing and Mechanism**

**Javed I. Moodi and Jyothi C. Abbar\***

*BMS Institute of Technology and Management, Bengaluru, 560119, Affiliated to Visvesvaraya Technological University, Belagavi, Karnataka  
E-mail : win.javed@gmail.com*

An antispasmodic myorelaxant drug, Chlorzoxazone was detected using a novel fabricated carbon paste electrode (CPE). The electrode fabrication involved the incorporation of nanostructured zirconium oxide ( $\text{ZrO}_2$ ) nanoparticles enhanced with the surfactant cetyltrimethylammonium bromide (CTAB). The Chemical composition of the hydro thermally synthesized zirconium oxide nanoparticles ( $\text{ZrONp}$ ) was studied by XRD and the surface morphology of the fabricated electrodes were studied using SEM and EDS measurements. Electroanalytical techniques like Cyclic voltammetry (CV), square wave voltammetry (SWV) were employed to develop insights on the electrocatalytic activity of the sensing surface. The modified sensing electrode demonstrated a selective and sensitive response to CHZ in a phosphate buffer solution at pH 7.0, showing significantly enhanced electro-catalytic activity compared to the bare CPE. The electron transfer reaction produced a diffusion-controlled mechanism. The linearity for the detection of CHZ was studied at SWV under optimum conditions and the range was found to be at 8.0 - 100.0  $\mu\text{M}$  with the LOD and LOQ values of 33.37 nM and 111.2 nM respectively. The



study utilized various excipients to examine their potential interference in the analytical process. The results demonstrated the simplicity of the method, with its high sensitivity and selectivity, in the determination of CHZ in real samples like urine and water.

### **AEO-10: Photocatalytic Degradation of Pharmaceutical Waste Lincomycin By Graphitic Carbon Nitride doped $\text{Co}_{0.5}\text{Ni}_{0.5}\text{Fe}_2\text{O}_4$ Nanocomposite**

**Sameeksha S. Patil and Kiran Thabaj**

*Department of Chemistry, Centre for Nanoscience and Nanotechnology, KLS Gogte Institute of Technology (Autonomous), affiliated to Visvesvaraya Technological University, Belagavi, Karnataka  
E-mail : sameekshapatil1008@gmail.com*

Managing water contamination due to rapid industrial development and urbanization will be a challenging task. Access to clean water is essential for public health, yet the rising pollutants such as pharmaceuticals in aquatic systems poses a significant challenge to effective water treatment. Conventional treatment methods such as adsorption, coagulation, membrane filtration, and advanced oxidation processes are used to treat pharmaceutical waste. Nanocomposite-based photocatalysts have gained significant attention due to their enhanced surface area, stability, and superior charge separation efficiency. Pharmaceutical waste, Lincomycin belongs to the antibiotics and its residues are easily spread in the environment because of its physicochemical properties. Despite growing interest in photocatalytic treatments for antibiotics, targeted studies on lincomycin remain scarce. In this study graphitic carbon nitride doped  $\text{Co}_{0.5}\text{Ni}_{0.5}\text{Fe}_2\text{O}_4$  nanocomposite is synthesized and characterized by SEM, TEM, BET analysis. These techniques conformed that  $\text{Co}_{0.5}\text{Ni}_{0.5}\text{Fe}_2\text{O}_4$  was effectively supported by Graphitic Carbon Nitride. The photocatalytic degradation of lincomycin was systematically studied by varying solution pH (3–11pH), catalyst dosage (0.1–1.0 g/L), and spiked drug concentration (5–50 mg/L) under UV (254nm and 366nm) and Visible irradiation. The results revealed that degradation efficiency strongly depended on these parameters, with optimum removal achieved at higher pH.

### **AEO-11: Assessment of Heavy Metal Accumulation in Water Hyacinth Along the Yamuna River: Seasonal Trends and Environmental Implications**

**Poonam Verma and Vinod Kumar**

*Department of Chemistry, Agra College, Dr B.R.A. University, Agra-282004  
E-mail : poonamverma3jan@gmail.com; vinodkchem@gmail.com*

The present study investigated the potential of water hyacinth

(*Eichhornia crassipes*) as a phytoremediator for the removal of heavy metals and the restoration of water quality in the Yamuna River within the regions of Mathura, Agra, Firozabad, and Etawah (Uttar Pradesh, India). Sampling was conducted during two seasonal regimes i.e. pre-monsoon and post-monsoon, covering the period from June to December 2023. The analysis revealed the presence of hazardous trace metals such as cadmium (Cd), chromium (Cr), copper (Cu), manganese (Mn), nickel (Ni), lead (Pb), and zinc (Zn) in the aquatic ecosystem of the Yamuna River. The primary sources of these contaminants were identified as industrial effluents, uncontrolled urbanization, and diverse anthropogenic activities. Heavy metal concentrations in water hyacinth tissues were found to be significantly higher during the pre-monsoon season due to the lower dilution capacity and reduced water flow. In contrast, post-monsoon concentrations were comparatively lower due to rainfall-induced flow that facilitated dispersion and partial flushing of pollutants. Despite these seasonal variations, the detected metal concentrations exceeded the permissible limits for drinking water established by the Bureau of Indian Standards (BIS) and the World Health Organization (WHO). The finding indicates that *E. crassipes* serves both as a phytoremediator and a bioindicator, highlighting its dual role in mitigating heavy metal pollution and monitoring riverine health. The study emphasizes the urgent need for governmental intervention to improve the water quality of the Yamuna River to safeguard aquatic ecosystems and public health.

## **AEO-12: Improvised Deposition of Prussian Blue on Stainless Steel by Spray Pyrolysis Technique for Catalyst OER Reaction**

**Kalpesh Tambe<sup>1, 2</sup>, Sudipa Manna<sup>1,2\*</sup> and Ashis Kumar Satpati<sup>1, 2\*</sup>**

<sup>1</sup>*Analytical Chemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085*

<sup>2</sup>*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094*  
E-mail : [asatpati@barc.gov.in](mailto:asatpati@barc.gov.in)

Porous thin films and nano layered interfaces have significantly higher importance in modern age's high energy demand. Surface porosity increases the charge storage and conversion efficiency due to enhancement of surface area for charge transfer reaction. Modified stainless steel surfaces developed by deposition techniques indigenously developed spray pyrolysis set up was used for the deposition of the Prussian blue films and the deposited electrode was used for the catalyst oxygen evolution reaction. Variation of films thickness and deposition temperature have strong influence on the catalytic

performance. The temperature was varied from 400 to 800 °C and the film thicknesses varied in the range of 50-1000 nm.

The Prussian Blue ( $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$ ) thin films were successfully deposited on stainless steel substrates using the upward spray pyrolysis technique and the electrocatalytic OER process was investigated using the films, the films generated at 700 °C found to performed better. The method enabled uniform, porous, and crystalline film formation through solution atomization, transport, evaporation, decomposition, and subsequent film growth. Increasing temperature led to enhanced crystallinity, as observed from the rising XRD peak intensity at  $50.9^\circ$  and the catalytic performance was decreased. Raman spectra exhibited a strong Fe–CN–Fe vibration at  $2148/\text{cm}^{-1}$  along with additional bands near 2085, 2156, 530, and  $274/\text{cm}^{-1}$  indicating the characteristic framework of Prussian Blue. Optical measurements and contact angle analysis revealed improved surface hydrophilicity at 700 °C, correlating with higher porosity and charge transfer efficiency. Electrochemical studies using cyclic voltammetry in KOH electrolyte (Hg/HgCl<sub>2</sub> reference) showed a significant increase in catalytic current density above 0.55/ V over multiple cycles, nearly tenfold higher than bare stainless steel. The results on the electrochemical investigation are shown in Figure 1. Kinetic studies confirmed an adsorption-controlled oxidation process, while chronoamperometry and chronopotentiometry demonstrated excellent stability. The results highlight that upward spray pyrolysis provides an efficient, scalable route to design porous, earth-abundant Prussian Blue electrodes for high-performance oxygen evolution reaction (OER) catalysis.

### **AEO-13: Microwave-Derived N-Doped CQDs as a Fluorescent Probe for Selective Bi<sup>3+</sup> Ions Detection via ‘Turn-Off’ Response**

**Anoushka<sup>1\*</sup>, Manviri Rani<sup>2</sup> and Uma Shanker<sup>1</sup>**

<sup>1</sup>*Department of Chemistry, Dr. B.R. Ambedkar National Institute of Technology Jalandhar, Barnala-Amritsar Bypass Road, Jalandhar, Punjab-144011*

<sup>2</sup>*Department of Chemistry, Malaviya National Institute of Technology Jaipur, Jaipur, Rajasthan 302017*

*E-mail : anoushka.cy.23@nitj.ac.in*

The increasing use of bismuth in various industries and pharmaceuticals has raised concerns about its environmental buildup and potential neurotoxic and nephrotoxic effects on humans. Existing methods for bismuth detection are often complex and expensive, highlighting the appeal of carbon quantum dots (CQDs) as a low-cost, low-toxicity, and easy-to-synthesize alternative. This study developed a novel, environmentally friendly one-pot microwave-assisted approach

for synthesizing nitrogen-doped carbon quantum dots (N-CQDs) for the selective and sensitive detection of bismuth ions ( $\text{Bi}^{3+}$ ). The N-CQDs demonstrated a high quantum yield of 47.5% and exceptional stability, making them effective fluorescent sensors for  $\text{Bi}^{3+}$  detection via fluorescence quenching. The detection limit was determined to be 0.365  $\mu\text{M}$  within a linear concentration range of 0.95–61.5  $\mu\text{M}$ , with the quenching mechanism attributed to dynamic quenching through a photoinduced electron transfer (PET) process. The practical application of this sensing system was validated using real-world samples, such as tap water, industrial wastewater, and agricultural runoff, with recovery rates ranging from 98.7% to 101.6%. Additionally, the versatility of these N-CQDs was showcased in applications like fluorescent ink and anti-counterfeiting. This method stands out for its simplicity, cost-effectiveness, and scalability. It provides a sustainable and efficient solution for detecting  $\text{Bi}^{3+}$  ions in diverse environmental settings and marks a significant advancement in metal ion sensing technologies.

#### **AEO-14: Evaluation and Comparative Study of Organochlorine Pesticide Residues in Seasonal Fruits and Vegetables by GC-MS and GC-ECD using QuEChERS Method**

**Dheeraj Kumar<sup>1</sup>, Nisha Singh<sup>2</sup> and Bhoopendra Singh<sup>3</sup>**

<sup>1</sup>Dept. of Chemistry, K.R. (PG) College, Mathura

<sup>2</sup>Dept. of Chemistry, Agra College, Agra

<sup>3</sup>Dept. of Chemistry, Agra College, Agra

E-mail : nishasingh9411604599@gmail.com

People in India are over scared for toxicity of vegetables & fruits, because the educational level of the farmers is not up to the mark. Farmers apply pesticides randomly on agricultural fields without maintaining pre-harvest intervals and dose. Majority of the farmers are unaware of pesticide types, level of poisoning, safety precautions and potential hazards on health and environment. Fruits and vegetables have nutritional value, but they can also be source of toxic contaminants such as pesticide residues. The aim of this study was to evaluate the concentration of organochlorine pesticide in seasonal fruits and vegetables purchase from sikandra mandi agra. The constant use of pesticides contaminated fruits and vegetables pose a leading threat to public health. Gas chromatography equipped with electron capture detector (GC-ECD) and Gas Chromatography - Mass Spectrometry (GC-MS) were used to monitor organochlorine pesticides

including 2,4,5,6-tetrachloro-m-xylene, heptachlor epoxide, chlordane, dieldrin, endrin aldehyde, endosulfan sulfate, methoxychlor and endrin ketone in ten different seasonal fruits and vegetables (tomato, chilly, cauliflower, pointed gourd, okra, peach, guava, banana, pear and pomegranate). However, the concentrations of estimated pesticides were less than the maximum residue limit values. But, the regular eating of pesticide infected fruits and vegetables may create serious health problems. The results of study indicated the need for strict guideline and regular monitoring of banned pesticide residues in fruits and vegetables to protect consumer's health.

## **AEO-15: Cu-MOF-Derived (Cu) TiO<sub>2</sub> Photocatalyst: Defect Evolution Studies and Enhanced Seawater Hydrogen Generation under Broad Solar Light**

**Nithin Kumar Banoth<sup>1,2</sup>, Bhavya Jaksani<sup>1,2</sup> and Ujjwal Pal<sup>1,2\*</sup>**

<sup>1</sup>*Department of Energy & Environmental Engineering, CSIR-Indian Institute of Chemical Technology, Hyderabad-500007*

<sup>2</sup>*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002*  
E-mail : [ujjwalpal@iict.res.in](mailto:ujjwalpal@iict.res.in); [upal03@gmail.com](mailto:upal03@gmail.com)

The stability of photocatalysts for solar-driven water splitting—particularly under the complex salinity conditions of seawater—remains a critical challenge. In this study, we investigate a metal–organic framework (MOF)-derived, defect-rich, copper-incorporated TiO<sub>2</sub> (M-CuTiO<sub>2</sub>) photocatalyst to elucidate its local structural dynamics during seawater-based hydrogen evolution under natural sunlight. The incorporated Cu sites markedly influence photocatalytic performance through valence-state fluctuations and associated phase transitions, while defect modulation within the TiO<sub>2</sub> lattice further governs activity. Notably, a simple catalyst film demonstrates substantially higher hydrogen production compared to the dispersed photocatalyst, underscoring the importance of efficient interfacial contact. Long-term stability is shown to be governed more by external operational factors—such as electron donor availability and solar intensity—than by intrinsic structural changes. The M-CuTiO<sub>2</sub> composite achieves sustained hydrogen generation of 5.5 mmol g<sup>-1</sup> h<sup>-1</sup> over 10 days in simulated seawater without the need for any sacrificial agent (Fig. 1). Complementary theoretical analysis indicates that adsorption of seawater cations strongly influences catalytic behavior by altering the solid–liquid interfacial environment. Overall, these findings provide key insights for the development of noble-metal-free, MOF-derived, and scalable photocatalysts for future industrial seawater hydrogen production technologies.

## **AEO-16: Pd-Bi Bimetallic Alloy on ZIF-8 Derived ZnO for Photocatalytic CO<sub>2</sub> to Methanol Production**

**Bapan Biswas<sup>1,2</sup>, Nithin Banoth<sup>1,2</sup>, Saad Mehmood<sup>1,2</sup> and Ujjwal Pal<sup>1,2\*</sup>**

<sup>1</sup>*Department of Energy and Environmental Engineering, CSIR-Indian Institute of Chemical Technology, Hyderabad-500007*

<sup>2</sup>*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002*

*E-mail: biswasbapan656@gmail.com; ujjwalpal@iict.res.in; upal03@gmail.com*

Solar-driven CO<sub>2</sub> reduction offers a sustainable route to produce value-added fuels. In this study, we engineered Pd–Bi bimetallic nanoalloys onto defect-rich ZnO derived from ZIF-8. The controlled chemical-reduction process yields a highly active heterostructure for selective CO<sub>2</sub>-to methanol conversion. Microscopic analyses confirm uniformly dispersed monoclinic Pd-Bi nanoalloy whose growth is governed by the reduction-potential disparity of Pd<sup>2+</sup> and Bi<sup>3+</sup>. XPS, PL, and EPR studies reveal that alloy effectively modulates surface defect states, suppresses electron-hole recombination, and establishes strong interfacial electronic coupling with ZnO. The optimized catalyst achieved remarkable methanol yield of 1984 μmol g<sup>-1</sup> with an apparent quantum yield of 0.87% under 4 hours of visible-light irradiation, nearly double that of pristine ZnO. Spectroscopic analyses confirmed strong interfacial electronic coupling, suppressed electron-hole recombination, and synergistic charge redistribution between Pd and Bi. Density functional theory calculations demonstrated enhanced CO<sub>2</sub> adsorption and favourable thermodynamic pathways for methanol formation, proceeding through stabilized oxygenated intermediates. The catalyst exhibited excellent stability across multiple catalytic cycles. This work establishes a versatile strategy for engineering alloy-decorated, MOF-derived semiconductor heterostructures for solar-driven carbon utilization, advancing scalable photocatalytic fuel production technologies.

## **AEO-17: Assessment of Bio-Based Epoxy Curing Systems for Aluminum-to-Aluminum Bonding Against the Conventional Curing System**

**Kishor Rajdeo\* and Krunal Trivedi**

*\*Henkel Product Development & AMP; Innovation Centre, Henkel Adhesives Technologies India. Private Limited, Survey No. 234, 235 and 245, Phase 1, Hinjewadi, Pune - 411 057*

*E-mail: kishor.rajdeo@henkel.com*

The mobility industry is continuously advancing, with increasing demand for lightweight materials possessing high strength, low density, and excellent corrosion resistance. These requirements are largely met by aluminum-based structures, driving their widespread adoption. In this study, two different sustainable: bio-based epoxy curing systems



were investigated for the formulation of epoxy adhesives for aluminum-to-aluminum bonding and were compared with a conventional fossil-based curing system. The influence of curing agent type on mechanical properties and thermal stability was systematically evaluated. Physical, mechanical, functional, and thermal characterizations were performed using a Brookfield viscometer, universal testing machine, Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and differential scanning calorimetry (DSC). The results demonstrate that adhesives formulated with bio-based curing systems exhibit key mechanical and thermal properties comparable to those of conventional curing systems. Therefore, bio-based curing agents present a promising and sustainable alternative for adhesive applications in the rapidly expanding industrial landscape.

### **AEO-18: Eco-Friendly Zinc Oxide Nanoparticles from Punica Granatum Leaf Extract: Green Chemistry for Photocatalytic Breakdown of Coomassie Blue R-250 Dye**

**Mallikarjunagouda B. Patil**

*Bharat Ratna Prof. CNR Rao Research Centre, Basaveshwar Science College, Bagalkot-587101, Karnataka*  
E-mail: mallupatil04@gmail.com

Because zinc oxide (ZnO) nanoparticles have numerous applications, many different methods of producing ZnO have been investigated. The most recent of these is the green chemistry strategy. In the current study, ZnO nanoparticles were synthesised using a green synthesis methodology that included the use of extract from the Punica granatum plant's leaf. To investigate the physicochemical properties of ZnO nanoparticles, advanced analytical methods such as UV-visible spectrophotometer, The techniques of Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), energy dispersive X-ray spectroscopy (EDAX), and scanning electron microscopy (SEM) were employed. In a UV-Vis spectrophotometer, ZnO nanoparticles showed a sharp absorption peak at 400 nm. XRD analysis reveals the shape and crystalline structure of ZnO. The surface morphology was examined using SEM, and the structure formation was verified using EDAX. The photocatalytic degradation of Coomassie brilliant blue R-250 dye (CBB\_ R-250) with green produced ZnO nanoparticles was also investigated. The results show that the green produced ZnO nanoparticles effectively degraded the Coomassie bright blue R-250 dye. Our study into the production of green photocatalysts for the removal of hazardous dyes from water has advanced as a direct outcome of this breakthrough.

## **AEO-19: Development and Validation of UV Spectrophotometric and RP-HPLC Methods for Quantification of Oseltamivir in Bulk and Tablet Dosage Forms**

**M.R. Pradeep Kumar**

*Department of Pharmaceutical Chemistry, KLE College of Pharmacy, Hubballi-580031. (A Constituent unit of KAHER Belagavi, Deemed-To-be-University)*

*Karnataka*

*E-mail: pradeepundefined5@gmail.com*

Oseltamivir phosphate (OP) is an antiviral drug used to treat influenza A and B by inhibiting the neuraminidase enzyme, which is essential for the release of viral particles. It is administered as an ester prodrug and later converted into its active form in the body. This study focuses on the development and validation of simple, accurate, and sensitive analytical methods—UV spectrophotometry and reversed-phase high-performance liquid chromatography (RP-HPLC)—for the estimation of Oseltamivir Phosphate in pharmaceutical formulations, following ICH guidelines.

## **AEO-20: Neutron Shielding Behaviour of Epoxy Composites Reinforced with hBN, GNP, Hybrid hBN and GNP Fillers.**

**Prashant N. Patil<sup>1</sup>, M. M. Hosamani<sup>2</sup>, N. R. Banapurmath<sup>3</sup>, Ashok M. Sajjan<sup>3</sup>, N. H. Ayachit<sup>1</sup>, and N. M. Badiger<sup>1\*</sup>**

<sup>1</sup>*School of Advanced Sciences, KLE Technological University, Hubballi-580031*

<sup>2</sup>*Department of Physics, M. S. Ramaiah University of Applied Sciences, Bengaluru-560058*

<sup>3</sup>*Centre for Materials Science, KLE Technological University, Hubballi-580031*

*E-mail: nbadiger@gmail.com; prashant.patil@kletech.ac.in;*

*patilputtu179@kletech.ac.in*

Lightweight polymer matrix composites are attractive for neutron shielding since hydrogen-rich epoxy resins provide strong moderation of fast neutrons. This work evaluates theoretical neutron transport properties of epoxy composites with graphene (GNP) and hexagonal boron nitride (hBN) fillers. Rule-of-mixtures densities were calculated: neat epoxy is 1.15/ gcm<sup>-3</sup>, epoxy plus 1-3/ wt% GNP are  $\approx$  1.15-1.16/ gcm<sup>-3</sup>, while hybrids with 9-27/ wt% hBN (plus 1-3/ wt% GNP) range  $\approx$  1.19-1.33/ gcm<sup>-3</sup>. Fast neutron removal cross sections ( $\Sigma_R$ ) and moderation power (MP) both decrease slightly with GNP loading, indicating moderation than neat epoxy. Thermal neutron absorption (1/e depth) is essentially unchanged or slightly increased by pure GNP (163-165/ cm vs 163/ cm for epoxy), confirming carbon's negligible capture ability. In contrast, hBN-GNP hybrids exhibit dramatically



enhanced thermal absorption:  $1/e$  depths drop to  $\approx 0.17\text{--}0.55/\text{cm}$  and total cross sections rise to  $\sim 2.5\text{--}6.7/\text{cm}^{-1}$  (neat epoxy  $\approx 0.67/\text{cm}^{-1}$ ). These changes are dominated by  $^{10}\text{B}$  in hBN. These analysis show that epoxy plus GNP composites do not improve neutron shielding, whereas epoxy along with hBN plus GNP hybrids provide excellent thermal neutron attenuation (through  $^{10}\text{B}$  capture) along with modest density increases (up to  $\sim 1.33/\text{gcm}^{-3}$ ). The results underscore GNP's limited role in shielding and hBN's key role as a neutron absorber.

### **AEP-CYSA-01: Electrochemical Investigation of Mercury Ions using Modified Pencil Graphite Electrode as A Sensor**

**Aishwarya K.G. and Y. Arthoba Nayaka\***

*<sup>1</sup>Department of P.G Studies and Research in Chemistry, Kuvempu University, Shankaraghatta 577451, Shivamogga, Karnataka  
E-mail : aishwaryakg568@gmail.com; drarthoba@gmail.com*

This study reports the development of a sensitive electrochemical sensor for the detection of mercury ions ( $\text{Hg}^{2+}$ ) using a pencil graphite electrode (PGE) modified with sodium lauryl sulphate and polymerized alanine (SLS@ALA/PGE). The electrode was fabricated by drop-casting SLS onto the alanine-polymerized PGE surface. Surface morphology and composition were examined using SEM, EDX, and EIS analyses. Compared to BPGE and ALA/PGE, the SLS@ALA/PGE electrode showed enhanced electrocatalytic activity toward  $\text{Hg}^{2+}$  ions, with higher peak currents and a slight negative shift in peak potential. The electrochemical behavior was systematically studied using CV, LSV, and DPV to evaluate the effects of polymerization cycles, pH, scan rate, concentration and selectivity. The sensor displayed a wide linear range ( $1.0\text{--}8.0\ \mu\text{M}$ ) with a low detection limit of  $4.46 \times 10^{-8}\ \text{M}$ . It also demonstrated high stability, reproducibility, and rapid electron transfer. Validation through water sample analysis confirmed its applicability and reliability for practical  $\text{Hg}^{2+}$  detection.

### **AEP-CYSA-02: Graphene Flakes Modified Carbon Paste Electrode as A Sensitive Electrochemical Sensor for the Quantification of Dopamine Agonist Drug Pramipexole in Biological Samples**

**Roshal C. Paul, Preemal N. Rodrigues and Ronald J. Mascarenhas\***

*Electrochemistry Research Group, Department of Chemistry, St Joseph's University, Bangalore, 560027  
E-mail: ronaldmasc@sju.edu.in*

A highly sensitive electrochemical sensor was developed using graphene flakes (GF) modified carbon paste electrode for detecting

pramipexole (PMXL), a dopamine agonist used in the treatment of Parkinson's disease and restless legs syndrome. Material characterization via X-ray diffraction (XRD), Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), and Raman Spectroscopy confirmed the layered, high-surface-area structure and crystalline integrity of the GF/CPE. Energy-dispersive X-ray (EDX) elemental analysis revealed a carbon-rich composition with minor oxygen/nitrogen doping. Electrochemical Impedance Spectroscopy (EIS) revealed a significant decrease in charge transfer resistance, indicating enhanced electron transfer kinetics at the surface of the GF-modified electrode. Cyclic Voltammetry (CV) further validated this enhancement, exhibiting a peak current response that was 3.16 times higher than that at the unmodified CPE. The optimal pH for detection was 3.0, ensuring immediate interaction between the analyte and the electrode. The GF/CPE sensor showcased two linearity ranges from  $1 \times 10^{-7}$  to  $1 \times 10^{-6}$  M and the other  $1 \times 10^{-6}$  to  $1 \times 10^{-5}$  M, with a remarkable limit of detection (LOD) of  $8.3 \times 10^{-8}$  M, and a limit of quantification (LOQ) of  $27.8 \times 10^{-8}$  M. This GF/CPE platform offers a cost-effective, eco-friendly, high-throughput alternative to chromatographic methods for therapeutic drug monitoring in clinical and pharmaceutical applications.

### **AEP-CYSA-03: Analytical Characterization of Aerosol Chemistry and Black Carbon Radiative Properties over Agra in the Indo-Gangetic Basin**

**Vaishnav Bartaria<sup>1</sup>, Auroop Ratan Ganguly<sup>3</sup>, Ashok Jangid<sup>2</sup> and Ranjit Kumar<sup>1</sup>**

<sup>1</sup>*Department of Chemistry, Faculty of Science, Dayalbagh Educational Institute Dayalbagh, Agra-282005*

<sup>2</sup>*Department of Physics and Computer Science, Faculty of Science, Dayalbagh Educational Institute, Dayalbagh, Agra-282005*

<sup>3</sup>*Civil and Environmental Engineering, College of Engineering, Northeastern University, Boston, MA 02115 (USA)*

*E-mail: vbartariya00@gmail.com; rkschem@rediffmail.com*

Severe aerosol loading across the Indo-Gangetic Basin (IGB) presents a complex analytical challenge due to the coexistence of chemically diverse particulate species from combustion, industrial, and secondary formation processes. This study develops an integrated analytical chemistry framework to quantify fine particulate matter (PM<sub>2.5</sub>) and black carbon (BC) characteristics using ground-based measurement and multi-spectral satellite datasets (MERRA-2, MODIS) and in-situ observations from a representative IGB site. Optical and compositional properties, including aerosol optical depth (AOD), single-scattering albedo (SSA), and absorption Ångström exponent (AAE),

were analyzed as chemical–optical descriptors of BC. The Beer–Lambert relation and Mie-theory inversion were employed to determine mass absorption coefficients (MAC) and complex refractive indices, key analytical indicators of aerosol composition and aging. Field samples analyzed through FESEM–EDX revealed agglomerated chain-like BC structures with submicron fractal geometry and heterogeneous mixing with sulfur- and nitrogen-rich compounds. Elemental spectra confirmed dominant carbonaceous and oxygenated components, along with trace metals (Fe, Si, Ca), indicating mixed combustion and crustal origins. Seasonal variations revealed enhanced BC concentrations during post-monsoon and winter, accompanied by secondary nitrate and organic aerosol enrichment, indicating atmospheric oxidation and surface functionalization. This study demonstrates how analytical chemistry tools can precisely resolve aerosol–radiation interactions, advancing understanding of short-lived climate pollutants in urban IGB environments and their broader environmental consequences.

### **AEP-CYSA-04 Carbon Quantum Dots Derived from Lablab Purpureus Peels and CuS<sub>2</sub> Nanocomposite Sensor for p-hydroxybenzoic Acid Detection in Cosmetic and Environmental Samples**

**Chanchal K. Sharma, Preemal N. Rodrigues and Ronald J. Mascarenhas\***

*Electrochemistry Research Group, Department of Chemistry, St Joseph's University, Bangalore, 560027  
E-mail: ronaldmasc@sju.edu.in*

Biogenic resources can be transformed into value-added products, providing economic and environmental benefits. Lablab purpureus peels, an agro-waste biomass rich in phytochemicals and biogenic elements, were used as a carbon precursor to synthesize carbon quantum dots (CQDs) through a hydrothermal process via a green method, which were combined with CuS<sub>2</sub> to form a nanocomposite (CuS<sub>2</sub>/CQDs). A CuS<sub>2</sub>/CQDs-modified carbon paste electrode (CPE) was developed for sensitive and selective detection of p-hydroxybenzoic acid (pHBA), a paraben associated with cancer and endocrine disruption. The surface morphology of CuS<sub>2</sub>/CQDs was characterized using Raman spectroscopy, Transmission electron microscopy (TEM), Field Emission scanning electron microscopy (FE-SEM), and X-ray diffraction. Electrochemical impedance spectroscopy (EIS) showed improved electron transfer kinetics at the modified electrode, with a two-fold increase in anodic peak current compared to bare CPE. Differential pulse voltammetry (DPV) revealed a linear detection range of  $1.0 \times 10^{-5}$  M to  $6.0 \times 10^{-6}$  M, with a detection limit of  $1.64 \times 10^{-7}$  M and limit

of quantification of  $5.49 \times 10^{-7}$  M. The sensor was successfully applied to real samples, including cosmetics (cream and lipstick) and water samples (lake and bore), demonstrating good selectivity, sensitivity, and reproducibility.

### **AEP-CYSA-05: Electrochemical Sensor for Detecting Hesperetin using Activated Carbon from Orange Peel Waste**

**Vaishnavi Vishwanath, P. N. Rodrigues and Ronald J. Mascarenhas**

*Electrochemistry Research Group, Department of Chemistry,  
St Joseph's University, Bangalore, 560027  
E-mail: vurs.09@gmail.com; ronaldmasc@sju.edu.in*

Dried orange peel, an abundant juice industry byproduct, was repurposed as a sustainable precursor for activated carbon, using phosphoric acid ( $\text{H}_3\text{PO}_4$ ) for activation. Scanning electron microscopy and X-ray diffraction confirmed that the resulting carbon possessed a well-defined structure suitable for sensing applications. The material was integrated into an electrochemical sensor for hesperetin, a health-promoting flavonoid found in citrus fruits. The sensor demonstrated high sensitivity, achieving a detection limit of 29.11 nM and exhibiting two linear response ranges (50 nM–1  $\mu\text{M}$  and 1  $\mu\text{M}$ –10  $\mu\text{M}$ ) via square-wave voltammetry. Reliable detection of hesperetin was maintained even in complex samples, with low interference from other flavonoids, enabling accurate quantification in orange peel extracts and human urine. During tests for simultaneous flavonoid analysis, only quercetin and hesperetin produced distinct signals; morin showed no interference. The sensor also exhibited consistent stability and reproducibility, highlighting its promise for practical analysis of flavonoids in real-world samples and reinforcing the value of upcycled orange peel in sustainable sensor development.

### **AEP-CYSA-06: Development and Evaluation of a $\text{WO}_3/\text{rGO}$ Enhanced Carbon Sensor for Improved Electrochemical Detection of Triclosan**

**Shreya S. Warad, Shweta J. Malode and Nagaraj P. Shetti\***

*Center for Energy and Environment, School of Advanced Sciences, KLE  
Technological University, Vidyanagar, Karnataka  
E-mail: shreyawarad5@gmail.com; npshetti@kletech.ac.in*

Triclosan (TCS) is a bactericidal agent recognized as a pollutant with potential endocrine-disrupting properties. Current research focuses on estimation of TCS in various biological and environmental matrices. This study introduces a novel sensor designed for the detection and analysis of TCS, utilizing a carbon paste electrode

modified with tungsten oxide (WO<sub>3</sub>) nanorods and reduced graphene oxide (rGO) nanocomposite in 0.2 M phosphate buffer solution (PB). Samples of fruits, vegetables, soil, and water contaminated with TCS pesticide were analyzed using square wave voltammetry in a phosphate buffer at pH 9.2. The developed sensor demonstrated significantly higher TCS oxidation currents than a standard carbon paste electrode. The nanostructured WO<sub>3</sub> enhanced the electrochemical response, leading to clearer peaks in the data. This research involved synthesizing a 1-D WO<sub>3</sub> nanostructure to facilitate TCS analysis. Characterization techniques, including SEM, XRD, TEM, and XPS, were employed to assess the material's crystallinity, morphology, and structural attributes. The synthesized 1-D WO<sub>3</sub> displayed a monoclinic crystal structure characterized by oxygen vacancies within its lattice. The study explored electrokinetic parameters such as the temperature effect, heterogeneous rate constant, scan rate, accumulation time, activation energy, pH levels, thermodynamic factors, and the number of electrons involved in the electro-oxidation of TCS.

### **AEP-CYSA-07: Voltammetric Determination of Thymol by a Modified Carbon Paste Electrode**

**H. R Sahana and Y. Arthoba Nayaka\***

*Department of Chemistry, School of Chemical Sciences, Kuvempu University, Shankaraghatta - 577451, Karnataka*

*E-mail : sahanahr0101@gmail.com; drarthoba@gmail.com*

The synthesised cerium-doped Fe<sub>2</sub>O<sub>3</sub> nanoparticles were used to develop a modified electrochemical sensor based on a carbon paste electrode (CPE) for the voltammetric determination of thymol(TML). The synthesised Fe<sub>2</sub>O<sub>3</sub> and Ce-doped Fe<sub>2</sub>O<sub>3</sub> NPs were characterized using XRD, FESEM with EDX, and TEM techniques. The average crystalline size of the synthesized nanoparticles has been found to be 19 to 30 nm. The Ce-Fe<sub>2</sub>O<sub>3</sub> modified carbon paste electrode (Ce-Fe<sub>2</sub>O<sub>3</sub>/CPE) exhibits superior electrochemical performance towards the oxidation of TML as compared to the Fe<sub>2</sub>O<sub>3</sub>/CPE. The Ce-Fe<sub>2</sub>O<sub>3</sub>/CPE exhibited a linear response towards the detection of TML under investigational conditions, with a detection limit of  $1.4052 \times 10^{-8} \text{M L}^{-1}$ . The various parameters such as heterogeneous rate constant ( $k^0$ ), number of electrons transferred ( $n$ ), electroactive surface area of the electrode ( $A$ ), and charge transfer resistance ( $R_{ct}$ ), have been calculated. The sensitivity, long-term stability, and reproducibility of the developed sensor were estimated. The analytical validity of the developed electrode has been examined through the real sample analysis using a soil sample.

## **AEP-CYSA-08: Ionic Liquid: Green Solvent for The Synthesis of Cellulose/Guar Gum/PVA Biocomposite**

**Nandkishor B. Shirsath\***

*Department of Chemistry, MGV's M.S.G. Arts, Science, and Commerce College, Malegaon, Savitribai Pule Pune University, Pune (MH)  
E-mail: shirsathnandkishor91@gmail.com*

In recent years, the development of clean, efficient and environmentally friendly chemical processes using less hazardous chemicals has been one of the main goals of researchers. Green chemistry and sustainability are directing the development of the next generation of biocomposite materials and products. Herein, the authors use the ionic liquid 1-butyl-3-methylimidazolium chloride ([BMIM]Cl) as a green solvent for the synthesis of biodegradable, biocomposite materials from cellulose (microcrystalline cellulose (MCC)), guar gum (GG) and poly(vinyl alcohol) (PVA). The effect of GG and PVA composition with MCC was evaluated by comparing the physical, chemical and mechanical characteristics of the produced biocomposite films with those of the regenerated cellulosic film. The tensile strength and hardness of biocomposite films is superior to that of the regenerated cellulosic film. In this method, [BMIM]Cl has been used as a solvent to dissolve and synthesize the MCC/GG/PVA biocomposite material. [BMIM]Cl is removed from the biocomposite material by washing it with ethanol and recovered by using a rotary evaporator. The synthesized biocomposite is an advanced biomaterial with several potential applications in packaging and other fields.

## **AEP-CYSA-09: Highly Sensitive and Colorimetric Detection of Mercury Ions in Water**

**R. Surya Sekhar Babu and Ravi Kumar Kanaparthi\***

*Department of Chemistry, Central University of Kerala, Tejaswini Hills, Periyar, Kasaragod, Kerala-671316.  
E-mail: rayudu.2301107009@cukerala.ac.in; rkchem@cukerala.ac.in*

Mercury is one of the highly toxic, bio-accumulating, and hazardous heavy metals that have adverse effects on various life forms. These adverse effects include enhanced risk for severe brain damage, kidney problems, immune dysfunction and motion disorders in humans. Considering the significance of mercury detection, a new molecular system B-1 has been designed and synthesized from carbamodithioate-based conjugated 1,3 Indanedione molecule-based sensor (B-1) for selective and rapid detection of mercury ( $Hg^{2+}$ ) in drinking water has been proposed. The B-1 molecule was synthesized by chemical reactions such as Vilsmeier-Haack and Knoevenagel condensation—further characterized by FT-IR, Mass spectrometry, NMR spectroscopy and



Single crystal XRD. In addition, photophysical properties were studied systematically using a UV-visible spectrometer and spectrofluorometer and TGA analysis was performed. Results showed that the sensor was thermally stable and exhibited strong absorption characteristics in the UV-visible region (200-550nm) and strong fluorescence in the range of (400-650nm). The sensor responds with a  $\text{Hg}^{2+}$  coordination interaction between (B-1) and  $\text{Hg}^{2+}$ . The thiol- $\text{Hg}^{2+}$  interaction was studied by fluorescence spectroscopy (bulk solutions) of (B-1) with increased concentrations of  $\text{Hg}^{2+}$  (10 nM to 30  $\mu\text{M}$ ). The sensor's specificity in the presence of other interfering metals like  $\text{Pb}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Na}^{2+}$ ,  $\text{Ag}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Pd}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Sn}^{2+}$  and  $\text{Cd}^{2+}$  has been determined. The sensor can be used as a highly sensitive, selective, portable, real-time, on-site  $\text{Hg}^{2+}$  optical probe for drinking water. We shall present photophysical studies as well as sensing applications of the new molecule, B-1.

### **AEP-CYSA-10: Development and Evaluation of Tamarind Gum/Sodium Alginate - ZnO Nanocomposite Microcapsules for Sustained Bioactive Release**

**Rakshith Nayak and Vishalakshi B.\***

*Department of Postgraduate Studies & Research in Chemistry, Mangalore University, Mangalagangothri, 574199 (DK), Karnataka  
E-mail : rakshithgavalkar96@gmail.com; vishalakshi2009@yahoo.com\**

A simple polymeric composite material in the form of microcapsules has been developed using tamarind seed gum, sodium alginate, and zinc oxide (ZnO) nanoparticles and evaluated as a matrix for sustainable release of bioactive agents in agrochemistry. The tamarind seed gum was interpenetrated into the sodium alginate matrix by an ionic gelation process achieved using calcium chloride. The physicochemical characterization of the formulated beads were carried out using FTIR, TGA, DTG, XRD and SEM. Swelling behaviour was investigated in an aqueous medium under various pH conditions. The composite beads were further examined for their capacity to deliver a natural pesticide (neem seed oil) and a nitrogen fertilizer (urea). The loading efficiencies were found to be 94.25% and 90.20% for neem seed oil and urea respectively, indicating excellent encapsulation potential of the microcapsules. Sustained release profile over 5-day period confirmed the slow-release nature. Release kinetics were analyzed using the Korsmeyer–Peppas model. The release exponent 'n' being is shown to be 0.5 indicating a Fickian diffusion-controlled mechanism. Antimicrobial assay demonstrated enhanced bacterial efficacy, primarily attributed to the presence of neem seed oil. This study highlights the

potential nanocomposite systems in developing eco-friendly, sustained-release platforms for sustainable agricultural practices.

## **AEP-CYSA-11: Electrochemical Analysis of Diclofenac, an Anti-inflammatory Drug**

**Pramod R. Vernekar<sup>1</sup> and Nagaraj P. Shetti<sup>2\*</sup>**

<sup>1</sup>*Center for Electrochemical Science and Materials, Department of Chemistry, K.L.E. Institute of Technology, Gokul, Hubballi-580027, Karnataka*

<sup>2</sup>*Center for Energy and Environment, School of Advanced Sciences, KLE Technological University, Hubballi-580031, Karnataka*

*E-mail: pramod.vernekar2@gmail.com; npshetti@kletech.ac.in*

A novel electrochemical carbon paste electrode sensor containing cobalt doped with tungsten oxide nanoparticles was developed for the detection of an anti-inflammatory drug, Diclofenac (DCFN). The electrode materials were characterized by scanning electron microscopy and X-ray powder diffraction. Electrochemical and square wave voltammetric techniques were employed to find the lowest limit of detection and quantification of DCFN. For the analysis, experiments were performed over the pH range of 3.0–11.2, but finally pH of 3.0 was found to be suitable for the analysis of DCFN in real samples of human urine as well as pharmaceutical dosage form.

## **AEP-CYSA-12: Visible-Light-Driven Fe-WSe<sub>2</sub> Photocatalyst for Simultaneous Hydrogen Generation and Industrial Dye Degradation**

**Ganga A. Muttagi, Madasu Sreenivasulu and Nagaraj P. Shetti\***

*Centre for Energy and Environment, School of Advanced Sciences, KLE Technological University, Hubballi-580031, Karnataka*

*E-mail : npshetti@kletech.ac.in*

One possible strategy for meeting the world's energy needs sustainably is the creation of hydrogen by photocatalytic water splitting. In the current work, we reported the synthesis and systematic optimization of a novel Fe-doped WSe<sub>2</sub> (Fe-WSe<sub>2</sub>) photocatalyst designed to improve the degradation of industrial dye and visible-light-driven hydrogen generation. The Fe-WSe<sub>2</sub> was synthesized through a hydrothermal method, successfully incorporating Fe into the WSe<sub>2</sub> lattice, which effectively tuned its electronic structure and improved light absorption and charge separation. The Fe-WSe<sub>2</sub> photocatalyst displayed a notable hydrogen evolution rate of 18.45 mmol g<sup>-1</sup>.h<sup>-1</sup><sub>(cat)</sub> under simulated solar irradiation, exceeding that of undoped WSe<sub>2</sub> (7.42 mmol g<sup>-1</sup>.h<sup>-1</sup><sub>(cat)</sub>) by more than twofold. Its n-type semiconductor properties, with a sufficiently negative flat band potential that enabled effective electron transport, were validated by band structure analysis and Mott-Schottky experiments. Furthermore, in visible light, Fe-



WSe<sub>2</sub> showed good photocatalytic degradation of Indigo Carmine dye, with over 93% clearance in 3 hours. This was due to longer charge carrier lifetimes and increased production of reactive oxygen species. Fe-WSe<sub>2</sub>'s dual-functional performance makes it a promising noble-metal-free photocatalyst for both sustainable energy generation and environmental remediation. This work offers a scalable method for using targeted doping techniques to increase the photocatalytic efficiency of transition metal dichalcogenides.

### **AEP-CYSA-13: A Novel Electrochemical Sensor for the Sensitive and Selective Detection of Dopamine Using ZIF-8/MgSnS<sub>4</sub>@GCN Nano-heterojunction**

**Sunith Kumar K.A.<sup>1</sup>, Bharath Kumar S.P.<sup>1</sup>, Rakshith G.N.<sup>1</sup>, Chetana S.<sup>2\*</sup> and Kumara Swamy N.<sup>1\*\*</sup>**

<sup>1</sup>*Department of Chemistry, JSS Science and Technology University, Mysuru-570006*

<sup>2</sup>*Department of Mechanical Engineering, ATME College of Engineering, Mysore-570028*

*E-mail: kumaryagati@gmail.com; chetana.s.mech@gmail.com; sunithkumar21ka@gmail.com*

Dopamine is a key catecholamine neurotransmitter and it has critical roles in the function of the human central nervous system. Abnormal release of dopamine is related to neurological diseases and depression. This makes it essential to develop a selective material that can detect Dopamine. Herein, a ZIF-8/MgSnS<sub>4</sub>@GCN nanocomposite is developed that detects the target analyte Dopamine. The nanocomposite was synthesized via the hydrothermal technique and later subjected to various kinds of material characterization, including X-ray diffraction, transmission electron microscopy, Raman, Brunauer-Emmett-Teller (BET) theory, FT-IR and energy-dispersive X-ray spectroscopy techniques. Upon confirming the formation of the nanocomposite, the material was evaluated for its selective detection of Dopamine using cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The glassy carbon electrode (GCE) was modified with ZIF-8/MgSnS<sub>4</sub>@GCN, resulting GCE/ZIF-8/MgSnS<sub>4</sub>@GCN exhibited excellent electrocatalytic activity, enabling excellent detection limit and quantification limit of 0.064 nM and 0.194 nM, with the corresponding sensitivities of 0.2651nM respectively. The real sample analysis showed excellent recovery rate assuring the GCE/ZIF-8/MgSnS<sub>4</sub>@GCN sensor for reliable detection of dopamine in pharmaceutical samples. Overall, ZIF-8/MgSnS<sub>4</sub>@GCN heterojunction acts as an excellent transducer material for electrochemical detection of dopamine.

## **AEP-CYSA-14: Electrochemical Sensing of Ciprofloxacin Using Poly (L-arginine) Modified Graphite Paste Sensor**

**Sharmila B.M. and J.G. Manjunatha\***

*Department of Chemistry, FMKMC College, A Constituent College of Mangalore University, Madikeri, Karnataka  
E-mail : manju1853@gmail.com*

In this current work, Cyclic Voltammetry (CV) method was employed to swiftly detect and analyze Ciprofloxacin (CF) using an electro polymerized poly (L-arginine) modified graphite paste sensor (PLMGPS). CF is an antibiotic that belongs to the class of drugs called quinolone and is widely used against bacterial infections. It is effective in preventing the bacterial growth or killing the disease-causing bacterial population. The excessive use of CF causes various mild and severe side effects like nausea, diarrhea, muscle weakness, renal failure etc. The surface morphology of the bare graphite paste sensor (BGPS) and PLMGPS was assessed through scanning electron microscopy (SEM) and electrochemical impedance spectroscopy (EIS). At optimal experimental conditions, the fabricated sensor exhibited a significantly low limit of detection (LOD) and showed high sensitivity towards CF in the presence of certain metal ions and organic interferents. Concurrent determination of CF with paracetamol (PT) was performed to authenticate the selectivity of CF and the outcome was observed to an acceptable extent without causing any hindrance for CF analysis. These experimental data specify that the designed sensor is able to detect CFX with appreciable results.

## **AEP-CYSA-15 : Drug-Templated In-Situ Electrochemical Synthesis of Fe-MOF/MWCNT Hybrids for Point-of-Care pH Sensing**

**Kondusamy Vignesh<sup>1,2</sup>, Ayyakannu Arumugam Napoleon<sup>2\*</sup> and Annamalai Senthil Kumar<sup>1,2\*</sup>**

*<sup>1</sup>Nano and Bioelectrochemistry Research Laboratory, CO<sub>2</sub> Research and Green Technologies Centre*

*<sup>2</sup>Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632 014*

*E-mail : askumar@vit.ac.in; askumarchem@yahoo.com*

Metal-organic frameworks (MOFs), a class of porous hybrid materials formed by coordinating organic linkers with transition-metal centers, have gained significant interest due to their tunable physicochemical properties and broad applications in chemistry, electrochemistry, and biomedicine. In this study, we report for the

first time the use of a nonsteroidal anti-inflammatory drug (NSAID), Etodolac (ETO), as a molecular template for the in situ electrochemical synthesis of Fe-MOF on multiwalled carbon nanotube (MWCNT) and other carbon-nanomaterial-modified electrodes in neutral phosphate buffer (pH 7). The resulting hybrid materials, denoted as MWCNT@Fe<sub>int</sub>-MOF and MWCNT@Fe<sub>ext</sub>-MOF, correspond to intrinsic and extrinsic Fe species, respectively. Comprehensive characterization by FE-SEM, FTIR, Raman, XRD, XPS, EQCM, and cyclic voltammetry confirmed that under anodic polarization at +1.0 V (vs. Ag/AgCl), Fe<sup>3+</sup> ions were electrochemically stripped from the electrode surface, while ETO was oxidized into a reactive dimeric intermediate, forming ETO-N-N-ETO linkages. These coupled processes promoted the growth of Fe-MOF architectures on the graphitic domains of carbon nanomaterials, yielding a unique hybrid organic-inorganic framework with excellent conductivity and Nernstian proton-coupled electron transfer (PCET) redox behavior at neutral pH. As a proof of concept, the MWCNT@Fe<sub>int</sub>-MOF-modified disposable three-in-one screen-printed electrode (SPE), integrated with a portable programmed potentiostat, enabled one-drop rapid pH sensing. The system was successfully validated with 15 real samples, showing <5% deviation compared to a standard pH meter. This work introduces pharmaceutical drugs as unconventional molecular templates for MOF synthesis, offering a new strategy for designing advanced electrochemical devices with superior sensing performance.

## **AEP-CYSA-16: Plant-Derived Betanin Immobilized on Carbon Black as a Redox-Active Green Electrode for Drift-Free Voltammetric and Potentiometric pH Sensing**

**Jayaprakash Meena<sup>1,2</sup>, Kanappan Santhakumar<sup>2\*</sup> and Annamalai Senthil Kumar<sup>1,2\*</sup>**

<sup>1</sup>Carbon Dioxide Research and Green Technology Centre, Vellore Institute of Technology University, Vellore 632 014

<sup>2</sup>Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology University, Vellore 632 014

E-mail: askumar@vit.ac.in; askumarchem@yahoo.com

Developing sustainable chemical strategies and low-carbon electrode materials is becoming central to next-generation electrochemical technologies. Plant-derived phytochemicals fit these goals well, yet understanding their intrinsic electron-transfer behavior and achieving stable, surface-confined redox systems remain demanding. In this work, an in-situ electrochemical reaction pathway is used to entrap redox-active betanin molecules directly from native beetroot

onto a carbon-black-modified glassy carbon electrode (GCE/CB@Betn-Redox) (Betn- betanin from beetroot) in a pH 2.2 KCl–HCl medium. Accessing native phytochemicals without extensive purification is typically challenging due to strong matrix effects, and conventional extraction methods involve multi-step separations. Unlike earlier reports describing the instability of betanin, the GCE/CB@Betn-Redox interface yields a robust and well-resolved proton-coupled electron-transfer signal at  $E^0 \approx 0.4$  V vs Ag/AgCl, with a surface-excess of  $17.02 \times 10^{-9}$  mol cm<sup>-2</sup>. A combination of physicochemical (TEM, FTIR, Raman), molecular (UPLC), and electrochemical (in-situ EQCM, SECM) analyses confirms the biomimetic electron-transfer capability of CB@Betn-Redox. A notable merit of this system is its non-mediated response toward common biochemical interferents, enabling selective pH transduction without the voltage drift typically associated with mediated redox processes. This stability and selectivity have been validated through voltammetric and potentiometric pH measurements, including tests with real sample matrices.

## **AEP-CYSA-17: Droplet Microfluidic Platform for Electrochemical Detection of Cadmium Ion**

**Badar Ali<sup>1,2</sup>, Khairunnisa Amreen<sup>1,3</sup>, Arshad Javed<sup>1,2</sup>,  
Satish Kumar Dubey<sup>1,2</sup> and Sanket Goel<sup>1,3</sup>**

<sup>1</sup>*MEMS, Microfluidics and Nanoelectronics (MMNE) Lab, Birla Institute of Technology and Science (BITS) Pilani, Hyderabad Campus, Hyderabad*

<sup>2</sup>*Department of Mechanical Engineering, Birla Institute of Technology and Science (BITS) Pilani, Hyderabad Campus, Hyderabad*

<sup>3</sup>*Department of Electrical and Electronics Engineering, Birla Institute of Technology and Science (BITS) Pilani, Hyderabad Campus, Hyderabad*  
E-mail : sgoel@hyderabad.bits-pilani.ac.in

Herein, cadmium ion detection, a predominant heavy metal ion, was accomplished in a droplet-based microfluidic platform using modified inkjet printed carbon paste electrodes (CPEs). Stable droplets were generated using optimized oil and surfactant concentrations, and flowrates. Electrochemical studies were performed in the potential range of  $-0.9$  to  $-0.6$  V. A linear range of  $400$ – $1200$   $\mu$ M was obtained with benchmarked LoD and LoQ values. Excellent reproducibility, repeatability, and minimal interference from co-existing ions were observed. Real sample analysis using the standard addition method showed  $<5\%$  error and good recovery. This study demonstrates electrochemical detection of in cadmium ions trapped droplets using surface roughness control, confirming the accuracy and reliability of the developed sensor.

## **AEP-01: Enhanced Photocatalytic Degradation of Congo Red Dye via CuO–N<sub>2</sub>O<sub>3</sub> Nanocomposites**

**Aakaash Dev Manwaal and K. Laxma Reddy\***

*Materials Chemistry Laboratory, Department of Chemistry, Osmania University, Hyderabad-500007, Telangana*  
*E-mail: aakaashdev.m@gmail.com; klreddy200542@gmail.com*

Synthetic dyes are responsible for around 20% of industrial water pollution. These dyes often persist in wastewater since many are not biodegradable, remaining in aquatic environments for decades and causing toxic effects that can bioaccumulate in the food chain. Even at concentrations as low as 1 mg/L, dyes color water, obstruct sunlight, and severely hinder photosynthesis for aquatic plants. This disruption lowers dissolved oxygen, raises biochemical and chemical oxygen demand, and damages the base of aquatic ecosystems. Many synthetic dyes are carcinogenic, mutagenic, and can trigger allergies or organ dysfunction in humans and wildlife. Photocatalysis, however, uses advanced materials like CuO–Nd<sub>2</sub>O<sub>3</sub> nanocomposites to harness light energy and break down dyes into harmless substances, offering efficient color removal with minimal secondary pollution. By converting hazardous dyes into non-toxic products, photocatalytic technologies present a promising route towards cleaner water and healthier ecosystems

## **AEP-02: Evaluation of Heavy Metal Concentrations in Groundwater and Associated Health Risks in Firozabad and Agra Districts**

**Dhirendra Yadav and Vinod Kumar\***

*Department of Chemistry, Agra College, Dr. Bhim Rao Ambedkar University Agra- 282004*  
*Email: dhirendrasnow@gmail.com; vinodkchem@gmail.com\**

Groundwater is an essential and vital component of any life support system. It is not only the basic need for human existence but also an essential input in all development activities. The present study aim to determine the concentrations of major and trace heavy metals (Li, Be, B, Na, Mg, P, K, Ca, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Mo, Cd, Pb) in 36 groundwater samples collected from different locations of Agra and Firozabad district blocks during pre-monsoon and post-monsoon seasons of 2023-24. To evaluate the groundwater quality for agricultural and drinking purposes, the HEI and the HPI were calculated. The concentrations of most HMs in the analyzed samples exceeded the permissible limits for routine use.

### **AEP-03: Ultra Sensitive Electro Sensing of Promethazine Hydrochloride in Biomedical and environmental samples using MoS<sub>2</sub>/Carbon Based Sensor**

**Mallika S. Wali<sup>1</sup>, Sharanappa T. Nandibewoor<sup>2</sup> and Ravindra R. Kamble<sup>1\*</sup>**

<sup>1</sup>*Department of Studies in Chemistry, Karnatak University Dharwad 580003*

<sup>2</sup>*Department of Chemistry, School of Advanced Sciences, KLE Technological University, Hubballi, 580031 Karnataka*

*E-mail: walimallika@gmail.com*

The first-generation antihistamine medication promethazine hydrochloride (PMZH) was detected with ultra sensitivity using a new electrochemical sensor built on MoS<sub>2</sub>/multi-walled carbon nanotube (MWCNT) composites. Employing a simple hydrothermal process, MoS<sub>2</sub> nanomaterial was obtained, and carbon nanotubes were added by the physical adsorption technique. Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Atomic Force Spectroscopy (AFM) and Scanning electron microscopy (SEM) in combination with Energy-dispersive X-ray spectroscopy (EDX), have all been used to characterise the materials. Electrochemical impedance spectroscopy (EIS) evaluated the performance of the materials. The electrochemical behaviour of PMZH at the electrochemical interface has been investigated using cyclic voltammetry (CV) and differential pulse voltammetry (DPV) utilizing various phosphate buffer conditions. The optimal results were found in the potential range of 0.1 V to 0.8 V at pH 7.0. The developed electrode exhibits a broad linear range (10nM to 3nM), superior sensitivity (0.39 nM), a low detection limit (1.31 nM), and outstanding selectivity and repeatability for PMH detection while operating in ideal conditions. Additionally, the modified GCE (MoS<sub>2</sub>/MWCNT/GCE) demonstrated a remarkable practical ability to detect PMH in pharmaceutical, biological, and water samples.

### **AEP-04: Eco-Friendly Synthesis and Antimicrobial Efficacy of Silver, Gold, and Copper Nanoparticles using Medicinal Plant Extracts**

**Aaquib Ahmad, Mahmood Shaikh and Khursheed Ahmed**

*MCE Society's Abeda Inamdar Senior College, Advanced Scientific Research Laboratory, Azam Campus, Pune-1*

*E-mail: Khursheedahmed@azamcampus.org*

In recent years, nanotechnology has emerged as a highly promising field, particularly in the eco-friendly synthesis of metal nanoparticles. This study reports the green synthesis of gold (AuNPs), copper (CuNPs), and silver nanoparticles (AgNPs) using plant extracts



of \*Gloriosa superba\*, \*Barleria prionitis\*, and \*Plumbago zeylanica\*, providing a sustainable and eco-friendly alternative to conventional chemical methods. The nanoparticles were characterized by UV–Vis spectroscopy, FTIR, SEM, and EDS, confirming their formation, crystalline nature, and nanoscale morphology. Their biomedical potential was evaluated through DPPH antioxidant assays, antimicrobial activity against \*Staphylococcus aureus\* and anticancer activity of CuNPs against MCF-7 cells. The phytochemicals in these medicinal plants act as natural reducing and stabilizing agents, highlighting an effective green approach for producing biocompatible nanoparticles with significant therapeutic potential.

### **AEP-05: A Visible-Light-Activated Metal-Doped TiO<sub>2</sub>/WO<sub>3</sub> Heterostructure Nano Photocatalyst for the Removal of Binary Dye Contaminants**

**Sandhya Rani Nayak and B.B.V. Sailaja**

*Department of Chemistry, Andhra University, Visakhapatnam, Andhra Pradesh, 530003*

*E-mail: sandhya04u@gmail.com, sailajabbv.chem@gmail.com*

This study presents, fabricated a mesoporous nanocomposite of metal-doped TiO<sub>2</sub>@WO<sub>3</sub> via a sol-gel method followed by a soaking treatment, designed to be active under visible light for the degradation of a dual-dye mixture. X-ray diffraction confirmed the presence of anatase TiO<sub>2</sub> alongside monoclinic WO<sub>3</sub> phases. UV-Vis diffuse reflectance spectroscopy demonstrated a narrowed bandgap, while TEM and BET examinations revealed a fine particle size and high specific surface area. SEM imaging showed spherical particles, smaller in size than those in undoped and solely metal-doped TiO<sub>2</sub> samples, and EDS (EDS) verified the elemental makeup. FTIR and XPS analyses validated that the metal ion had substituted into the TiO<sub>2</sub> lattice in place of Ti<sup>4+</sup>, and also confirmed the composite's formation; XPS further provided details of oxidation states, and XRF affirmed the elemental presence. Electrochemical impedance spectroscopy (EIS) and photoluminescence (PL) studies indicated suppressed electron-hole recombination and bandgap narrowing, underlining the enhanced optoelectronic behaviour of the nanocomposite. Under optimized conditions (catalyst dose, initial dye concentrations, pH) for Congo/Red and Brilliant/ Green dye degradation, the catalyst achieved approximately 96 % removal of Congo Red in 90 minutes and about 98 % removal of Brilliant Green in 80 minutes. Altogether, the metal-doped TiO<sub>2</sub>@WO<sub>3</sub> nanocomposite exhibits outstanding photocatalytic performance and shows strong potential for environmental remediation applications.

## **AEP-06: Pre-treated Glassy Carbon Electrode Sensor for Mycophenolate Mofetil**

**G.S. Sumanth, B.E. Kumara Swamy\*, K. Chetankumar and Puneeth**

*Department of P.G Studies and Research in Industrial Chemistry, Kuvempu University, Jnanasahyadri, Shankaraghatta -577451, Shivamogga (D), Karnataka*

*E-mail: kumaraswamy21@gmail.com; bek@kuvempu.ac.in*

By using cyclic voltammetry (CV) approaches, the electrochemical pre-treatment method was used to activate the glassy carbon electrode for the detection of mycophenolate mofetil. At the KOH-pretreated glassy carbon electrode for MMF, the effects of concentration, pH, and scan rate were investigated. It illustrates the adsorption-controlled technique and shows that the MMF had a good limit of detection of 1.87  $\mu\text{M}$ . In the simultaneous electroanalysis of MMF, the recommended electrode demonstrated good sensitivity and dependability. The produced electrode demonstrated a 92-95% recovery rate for the very sensitive and recoverable detection of MMF in actual samples.

## **AEP-07: $\text{Fe}_3\text{O}_4$ -Modified Mustard Cake Biomass as a Cost-Effective Solution for Dye-Contaminated Water**

**Kashika Tiwari and Priyanka Jain\***

*IIS (deemed to be a University), Jaipur, Rajasthan*

*E-mail: kashikatiwari2001@gmail.com; priyanka.chemistry@iisuniv.ac.in*

The present study reports the synthesis of a novel magnetized adsorbent derived from mustard cake for the efficient removal of crystal violet dye from aqueous solutions. Mustard cake, an agricultural by-product, was modified with  $\text{Fe}_3\text{O}_4$  to enhance its adsorption and magnetic separation properties. The prepared material was characterized using scanning electron microscopy (SEM) coupled with energy-dispersive X-ray analysis (EDX), confirming the successful deposition of  $\text{Fe}_3\text{O}_4$  on the biomass surface. Batch adsorption experiments revealed that the removal of crystal violet dye followed pseudo-first-order kinetics, with maximum removal efficiency ranging between 87–90%. Equilibrium data were well described by the Langmuir isotherm model, indicating monolayer adsorption on a homogeneous surface. In addition, adsorption behaviour was further validated through artificial neural network (ANN) modelling, which demonstrated strong predictive accuracy, highlighting its potential for process optimization. The results suggest that magnetically modified mustard cake is a cost-effective, sustainable, and reusable adsorbent for wastewater treatment applications.



## **AEP-08: Development of a Sustainable Halonanoclay–Carbon Paste Composite Electrode for Electrochemical Oxidation and Determination of Tryptophan**

**Jayant I. Gowda\***

*Department of Chemistry, BLDEA's Commerce, B.H.S. Arts and T.G.P. Science College, Jamkhandi-587301, Karnataka*

*Research Centre in Chemistry, BLDEA's Commerce, B.H.S. Arts and T.G.P. Science College, Affiliated to Bagalkot University, Jamkhandi-587301, Karnataka*

*E-mail: jayantgowda4@gmail.com*

This research aims to develop a sensitive electrochemical technique for detecting and quantifying Tryptophan (TRP), an amino acid, using a carbon paste electrode modified with halonanoclay. The morphology of the prepared electrode was characterized using XRD and SEM techniques. Tryptophan electro-oxidation was investigated primarily using cyclic voltammetry (CV). Systematic studies were conducted to explore the influence of various parameters, such as scan rate, pH, pre-concentration time, modifier quantity, and analyte concentration, on the peak current response of TRP. Tryptophan exhibited an irreversible, well-defined oxidation peak at 0.820 V. Cyclic voltammetry was used to evaluate the effect of scan rate, allowing for the determination of physicochemical parameters, including the heterogeneous rate constant ( $k^0$ ) and the number of electrons ( $n$ ) involved in the electrochemical reaction. Additionally, differential pulse voltammetry was employed to quantitatively analyze pharmaceuticals and human biological fluids. Linearity in detection was observed between  $2.0 \times 10^{-7}$  M and  $50.0 \times 10^{-6}$  M, with a limit of detection of  $7.77 \times 10^{-9}$  M. As a result, the current electrocatalytic method provides a quick, accurate, and simple method to detect TRP in biological medium and pharmaceutical formulations. A sensor with excellent reproducibility, short response times, and outstanding stability has been described as the modified electrode.

## **AEP-09: Electrochemical Properties of the Antimalarial Drug Chloroquine Phosphate at Silver Nanoparticles: A Voltammetric Method**

**Ankitha G.N.<sup>1</sup>, Rajeshwara Achur<sup>1</sup> and B.E. Kumara Swamy<sup>2\*</sup>**

<sup>1</sup>*Department of P.G. Studies in Biochemistry, Jnana Sahyadri, Kuvempu University*

<sup>2</sup>*Dept. of PG Studies and Research in Industrial Chemistry, Kuvempu University, Jnana Sahyadri Shankaraghatta - 577451, Shivamogga (D), Karnataka (S).*

*E-mail : kumaraswamy21@gmail.com; bek@kuvempu.ac.in*

The silver nanoparticles were synthesized using the coprecipitation method, and Energy Dispersive X-ray Spectroscopy (EDS), scanning

electron microscope (SEM), and X-ray diffraction (XRD) techniques confirmed the characterization of the prepared nanoparticles. The nanoparticles (NPs) were used for the electrochemical detection of chloroquine phosphate with cyclic voltammetry (CV) and differential pulse voltammetry (DPV) using a carbon paste electrode. The scan rate study indicates that the process was adsorption-controlled, and the pH study shows that there is an unequal sharing of protons and electrons. The DPV method was employed to analyze the concentration effects and interference, with results showing clear peak separation of CQP and CT (catechol) in a binary mixture. The Ag-modified electrode demonstrates good limits of detection (LOD) and quantification (LOQ), i.e., 4.482  $\mu\text{M}$  and 14.9  $\mu\text{M}$ , respectively. This study can be applied to assess the efficacy of other actual drug samples.

### **AEP-10: Heavy Metals Pollution Index (HPI) Assessment through Water Analysis for Yamuna River Water in Agra District (India)**

**Mukesh Chand<sup>1</sup>, Ravi Prakash<sup>2</sup> and R.B. Singh<sup>3</sup>**

<sup>1</sup>*Department of Sociology, B.S.A. College, Mathura-281004, U.P.*

<sup>2</sup>*Department of Chemistry, B.S.A. College, Mathura-281004, U.P.*

<sup>3</sup>*Scientist 'C' (UGC), Department of Zoology, School of Life Sciences*

*Dr Bhimrao Ambedkar University, Khandari Campus, Agra-282002, U.P.*

*Email: mcsharmasoc@gmail.com; drravichem@gmail.com;*

*rbsinghugc@gmail.com*

Rapid urbanization, industrialization and population growth in burgeoning cities has led to increased flux of heavy metals laden wastewater into India's rivers traversing through these cities. Heavy metals can enter river systems mainly from point and non-point sources i.e., effluents of industrial activities, domestic wastewater, runoff from agricultural fields and urban areas which supply huge quantities of inorganic ions and heavy metals. Heavy metals such as cobalt (Co), copper (Cu), chromium (Cr), iron (Fe), magnesium (Mg), manganese (Mn), molybdenum (Mo), nickel (Ni), selenium (Se) and zinc (Zn) are required to maintain various biochemical and physiological functions in living organisms when in very low concentrations, however, they become toxic when exceed certain threshold concentrations. The present study was conducted on heavy metal pollution index (HPI) of Yamuna river water in Agra district U.P. (India) at sites viz., A1, A2, A3, A4 and A5 for summer and post-rainy seasons. Mean concentration of heavy metals followed the order  $\text{Zn} > \text{Fe} > \text{Cu} > \text{Ni} \geq \text{Mn} > \text{Cr} > \text{Pb} > \text{Cd}$  in summer and  $\text{Zn} > \text{Fe} > \text{Mn} > \text{Cu} > \text{Ni} > \text{Cr} > \text{Pb} > \text{Cd}$  in postrainy seasons. Zn and Cu were within permissible limit for drinking water quality at all sites in both seasons. Fe, Zn, Cr and Mn increased during post-rainy season against their covalent

index. Mean heavy metal pollution index (HPI) for each sampling site reflected highest pollution at A4 site. Mean HPI for Yamuna river water in summer (261) decreased conspicuously in post-rainy season (92.5). Metal quality index (MQI) values were highest at A4 site i.e., 23.15 in summer and 22.0 in post-rainy seasons. Pearson's analysis showed significant positive correlation among all heavy metals.

## **AEP-11: Investigation of Time-Directed Transformation of Fibrous to Microspherical Architectures using Agro-Waste Cellulose PES Membranes for Emulsified Mixture Separation**

**Sowmya R.K.<sup>1</sup>, D.S. Aditya<sup>1</sup>, K.N. Santhosh<sup>1</sup>, A.B. Hemavathi<sup>2</sup> and S.K. Nataraj<sup>1\*</sup>**

<sup>1</sup>Centre for Nano & Material Sciences, JAIN University, Jain Global Campus, Bangalore-562112

<sup>2</sup>Department of Polymer Science and Technology, Sri Jayachamarajendra College of Engineering, JSS Science and Technology University, Mysore-570006  
E-mail: sk.nataraj@jainuniversity.ac.in; sknata@gmail.com

The rising environmental burden posed by emulsified waste engine oil in industrial effluents demands advanced separation platforms that combine efficiency with sustainability. In this study, a bio-derived membrane was fabricated via self-assembly of cellulose microspheres from waste areca husk. FESEM analysis revealed time-dependent morphological different transitions from fibrous fragments at 1 h to densely packed microspheres at 24 h membrane, indicating solvent-driven kinetic restructuring and microsphere formation influenced by dissolution time and cellulose chain mobility. P-XRD provided insight into the coexistence of crystalline and amorphous regions, highlighting the structural complexity of the assembled microspheres. Attenuated Total Reflectance Infrared (ATR-IR) spectroscopy confirmed the presence of cellulose-specific functional groups in modified membranes, validating the successful transformation of areca husk into microspherical architectures. This study demonstrates the pivotal role of solvent and dissolution time in tailoring the physicochemical properties of cellulose microspheres and reveals the viability of areca husk biomass as a sustainable source for cellulose-based functional engineered materials. Additionally, the application of these cellulose 24 h membrane is used in a continuous flow method for treating emulsified mixtures of waste engine oil with dyes. The 24 h membrane demonstrated impressive performance, achieving >98% rejection efficiency and a flux rate of 614 L.m<sup>-2</sup>.h<sup>-1</sup>, highlighting its potential for efficiently removing complex contaminant mixtures, including emulsified waste engine oil and dyes. This sustainable approach highlights the circular utilization of agro-waste, promoting low-impact

fabrication of bio-derived membranes for eco-efficient wastewater treatment and advancing green engineering for environmental remediation.

### **AEP-12: A Redox-Active Polymer Film on A Carbon Frame for Detection of an Anticancer Drug**

**Shikandar D. Bukkitgar and Nagaraj P. Shetti\***

*\*Centre for Energy and Environment, School of Advanced Sciences, KLE Technological University, Vidyanagar, Hubballi -580 031, Karnataka  
E-mail: sikhandar.db@kletech.ac.in; npshetti@kletech.ac.in*

Electrochemical techniques have recently proven to be a promising platform for monitoring human health and the environment. In the present study, an electrochemically polymerized carbon sensor is used for the detection of the anti-cancer drug 5-Fluorouracil. The AFM investigation suggested an increase in surface roughness, which enhances electrochemical activity and synergistically eases electron transfer kinetics by forming a conducting layer on the surface. The proposed method demonstrated a very low detection limit of 2.54 nM. Furthermore, the analytical characteristics of the electrode were investigated for interference, reproducibility, and repeatability. High recoveries were obtained from the pharmaceutical and human spiked urine samples, indicating that the proposed method was suitable for clinical trials.

### **AEP-13: Synthesis of Copper Nanoparticles as Efficient Catalysts for the Hydrogen Evolution Reaction**

**Tarannum S. Attar and Satish K. Pardeshi\***

*Department of Chemistry, Savitribai Phule Pune University (formerly University of Pune), Ganeshkhind, Pune-411007  
E-mail: satish.pardeshi@unipune.ac.in*

The rising demand for sustainable and clean energy technologies has intensified research into hydrogen generation. The shift towards sustainable hydrogen fuel necessitates the development of highly efficient, earth-abundance electrocatalysts to replace expensive Platinum (Pt). The development of highly efficient, earth-abundant electrocatalysts for the Hydrogen Evolution Reaction (HER) is critical for sustainable hydrogen production via water electrolysis. Copper nanoparticles (Cu NPs) have emerged as promising non-noble metal electrocatalysts for the hydrogen evolution reaction (HER) due to their earth-abundant, cost-effective, and favourable catalytic activity. Their catalytic activity toward HER was investigated in two different electrolyte media, 1 M KOH (alkaline) and 0.5 M Na<sub>2</sub>SO<sub>4</sub> (neutral).

Electrochemical measurements, including linear sweep voltammetry (LSV), cyclic voltammetry, and electrochemical impedance spectroscopy (EIS), revealed a marked dependence of HER efficiency on the electrolyte environment. The long-term durability of the catalyst was evaluated through chronoamperometric measurements. The study highlights the critical role of electrolyte composition in optimizing the performance of non-noble metal electrocatalysts, underscoring the potential of copper-based nanomaterials as low-cost, scalable catalysts for hydrogen production. The mechanistic insights clarifying the higher efficiency of 1 M KOH relative to 0.5 M Na<sub>2</sub>SO<sub>4</sub> are discussed. These findings demonstrate the potential of Cu NPs as efficient and low-cost electrocatalysts for sustainable hydrogen production in alkaline environments.

## **AEP-14: Green-Synthesized Nanocomposites for Enhanced Photocatalytic Environmental Remediation**

**Priyanka, Somya Chaudhary and Durgesh Raj Mohan**

<sup>1</sup>*Deptt. of Chemistry, Vidhyotma (P.G.) College, Khatauli, Muzaffarnagar*

<sup>2</sup>*Deptt. of Chemistry, Sanskriti University*

<sup>3</sup>*Deptt. of Chemistry, Maharaj Singh College, Saharanpur*

*E-mail: rajmscollege@gmail.com*

The growing demand for sustainable technologies has accelerated research on eco-friendly approaches to synthesize advanced nanomaterials. In this work, nanocomposites were synthesized via green routes employing plant extracts and other non-toxic precursors, thus eliminating the use of hazardous chemicals and minimizing environmental footprints. The synthesized nanocomposites were systematically characterized using XRD, UV-Vis, FTIR, SEM, and TEM analyses to evaluate their structural, optical, and morphological properties. Results revealed uniform particle distribution, reduced agglomeration, and strong interfacial bonding between the composite constituents. Photocatalytic performance was investigated under visible light irradiation, where the green-synthesized nanocomposites exhibited significantly enhanced photocatalytic activity for the degradation of organic pollutants in aqueous systems. The superior activity is attributed to the synergistic interaction between the composite components, improved band gap tuning, and efficient charge carrier separation, which collectively reduced electron-hole recombination. Moreover, the use of renewable bio resources in synthesis highlights the sustainability and scalability of the proposed method. This study demonstrates that green-synthesized nanocomposites not only ensure environmental safety but also provide promising alternatives to conventional catalysts for wastewater treatment, environmental

remediation, and clean energy applications. Such materials offer a pathway toward developing next-generation photo catalysts that integrate efficiency, stability, and sustainability.

### **AEP-15: Ambient Air Quality Monitoring of Nandurbar City during the Diwali Festival: A Case Study**

**Kalpesh C. Sawant, Ganesh N. Bagul, Tushar R Borane, Himmat A. Patil, Yogesh V. Marathe, M.R. Patil and V.S. Shrivastava\***

*Nano-Chemistry Research Laboratory, G. T. Patil College, Nandurbar-425412.  
E-mail: drvinod\_shrivastava@yahoo.com*

Ambient air quality monitoring was conducted at three selected locations in Nandurbar city to assess the impact of Diwali festivities on pollution levels. Key air quality parameters, including particulate matter (PM<sub>10</sub> and PM<sub>2.5</sub>), nitrogen dioxide (NO<sub>2</sub>), and sulfur dioxide (SO<sub>2</sub>), were monitored during pre-Diwali, Diwali, and post-Diwali periods. Eight-hour continuous air sampling for respirable suspended particulate matter (RSPM) and four-hour sampling for gaseous pollutants were carried out at each site. Real-time monitoring was supported with meteorological data to evaluate the influence of weather conditions on pollutant dispersion. Preliminary results indicate a sharp rise in particulate matter concentrations during the Diwali period, with PM<sub>10</sub> and PM<sub>2.5</sub> levels showing distinct spikes attributable to firecracker emissions. Similarly, elevated levels of NO<sub>2</sub> and SO<sub>2</sub> were observed, particularly during peak celebration hours. Statistical analysis confirms significant differences in pollutant concentrations between pre- and post-Diwali periods, highlighting the short-term but substantial impact of festival-related activities on ambient air quality.

### **AEP-16: Biowaste-Derived Cellulose/MOF Hybrid Membranes for Forward Osmosis: A Scalable Strategy for Complex Wastewater Treatment**

**Suhas Basagonda Kale, Aditya D.S., Santosh K.N., Dibyendu Mondal\* and S.K. Nataraj\***

*Sustainable Energy Materials and Processes Research Group, Centre for Nano & Material Science, Jain Global Campus, Jain University, Bangalore 562112  
E-mail : sk.nataraj@jainuniversity.ac.in*

The increasing need for sustainable and energy-efficient water treatment motivates the search for membrane materials that reduce dependence on petroleum-based polymers. In this study, agricultural biowaste was transformed into a high-value functional material for the development of forward osmosis (FO) membranes. Cellulose derived



from the biowaste was combined with Cu-BTC metal–organic frameworks (MOFs) to form a cellulose/MOF hybrid, which was subsequently embedded into a polyethersulfone (PES) matrix to fabricate freestanding thin-film nanocomposite FO membranes at different loadings. All materials and membranes were systematically characterized to confirm functional group integration, crystallinity, surface morphology, elemental distribution, and physicochemical properties. The incorporation of the cellulose/MOF hybrid significantly enhanced membrane hydrophilicity, surface charge, and porosity compared to the pristine PES membrane. Performance evaluation demonstrated that the optimized membrane exhibited substantially higher water flux and dye rejection efficiency in FO operation. Additionally, the membrane effectively treated real industrial wastewater, highlighting its practical relevance for resource recovery applications. This work provides a novel pathway for biowaste valorisation into advanced FO membranes while reducing polymer dependency. The results demonstrate that the cellulose/MOF hybrid not only enhances membrane performance, but also supports a circular-material model aligned with sustainable membrane manufacturing and the water energy nexus.

### **AEP-17: Cyclic Voltammetric Determination of Sunset Yellow at NiO nanoparticles Modified Carbon Paste Electrode**

**Radhika M.<sup>1</sup>, B.E. Kumara Swamy<sup>2\*</sup> and Anitha G.<sup>1</sup>**

<sup>1</sup>*Dept of Industrial Chemistry, Sahyadri Science College, Kuvempu University, Shivamogga (D) Karnataka(S).*

<sup>2</sup>*Dept of PG Studies and Research in Industrial Chemistry, Kuvempu University, Jnana Sahyadri Shankaraghatta (577451) Shivamogga (D) Karnataka(S).*

*E-mail: kumaraswamy21@gmail.com; bek@kuvempu.ac.in*

In the present work, NiO nanoparticles were prepared using the Co-precipitation method to detect Sunset Yellow (SY) a food dye. The prepared sample was characterized by XRD (X-ray diffraction) in addition to scanning electron microscopy (SEM) techniques. Current work shows the advancement of electrochemical sensors using cyclic voltammetry and differential pulse voltammetry. Different parameters like scan rate, pH study, interference, and simultaneous study of Uric acid (UA) in Sunset Yellow (SY) occurrence were carried out. DPV has a detection limit of 0.7283  $\mu\text{M}$  and a Quantification limit of 2.42  $\mu\text{M}$  at pH 7.4. The prepared electrode also obtained a stability value of 96.73 % for 15 cycles. The prepared NiO-modified carbon paste electrode shows promising electrochemical sensing for Sunset Yellow.

## **AEP-18: Graphitic Carbon Nitride-Based Electrochemical Platform for Direct and Sensitive Quantification of Pramipexole**

**S. Dhanalakshmi<sup>1</sup>, Shweta J. Malode<sup>2</sup> and Nagaraj P. Shetti<sup>2\*</sup>**

<sup>1</sup>*Department of Chemistry, School of Advanced Sciences, KLE Technological University, Vidyanagar, Hubballi-580031, Karnataka*

<sup>2</sup>*Center for Energy and Environment, School of Advanced Sciences, KLE Technological University, Vidyanagar, Hubballi-580031, Karnataka*  
E-mail: s\_dhanalakshmi@kletech.ac.in; dr.npshetti@gmail.com

Pramipexole (PMXL), a benzothiazole-based drug used to treat Parkinson's disease, can cause severe side effects at elevated levels, highlighting the need for sensitive trace-level detection. A voltammetric electrochemical sensor was developed for the quantification of PMXL using graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) as a functional electrode modifier. gCN was synthesized through high-temperature thermal condensation and characterized to confirm its morphology and structural features. Cyclic voltammetry (CV) showed a distinct anodic peak corresponding to PMXL oxidation, with the gCN-modified carbon paste electrode (gCN-CPE) exhibiting enhanced peak currents and a lower oxidation potential compared to the unmodified electrode. Parameter optimization demonstrated that PMXL oxidation follows a diffusion-controlled process involving equal numbers of electrons and hydronium ions. The gCN-CPE provided a broad linear range from 0.05 to 500  $\mu$ M and a low detection limit of 0.012  $\mu$ M within the working concentration range (0.5–30  $\mu$ M). Interference studies confirmed the sensor's good selectivity, and tablet analysis demonstrated its practical applicability. High recovery values further validated the accuracy and reliability of the developed method.

## **AEP-19: Synthesis of Zinc Oxide Nanoparticles by Cannabis Sativca and their Photocatalytic Applications**

**Somya Chaudhary and Durgesh Wadhwa**

*Department of Chemistry, Sanskriti University, Mathura*  
E-mail : rajmscollege@gmail.com

Biosynthesized metal oxide (MeO) nanoparticles (NPs) have triggered a huge global research interest owing to their advancement and various environment remediation, personal care products, medical, energy, sensing and water treatment applications. They demonstrate developing assets in various industries, remarkably with their heightened physiochemical, optical, mechanical and electronic attributes. The physical and chemical routes have been a sticking point in the production of MeO NPs, owing to the natural and



environmental risk linked with utilizing these approaches. The synthesis of ZnO NPs production via the biological method employing cannabis sativa as a precursor material for metal ion reduction. Hence, in this paper a biosynthesized approaches using plant extract (cannabis sativa) for ZnO NPs production and their applications for photocatalytic dye degradation were studied.

### **AEP-20: Biosensing of Brucine at a poly (L-tryptophan) Modified CNT Paste Electrode: Analytical Performance Evaluation**

**J.G. Manjunatha**

*\*Department of Chemistry FMKMC, College, Madikeri, Mangalore University  
Constituent College, Karnataka-571201  
E-mail: manju1853@gmail.com*

Assessing food safety and keeping an eye on human health depend on the development of a rapid, sensitive, and affordable brucine toxicity detection system. In this study an innovative electrochemical sensor was fabricated for the sensitive and selective determination of brucine (BC), based on a carbon nanotube paste electrode (BCNTPE) surface were improved by the electropolymerization of poly (L-tryptophan) (PTMCNTPE). This modified electrode enhances the electrochemical response of the examining molecule. The study was conducted using a cyclic voltammetry technique in phosphate buffer saline of physiological pH 3.0 at a scan rate of 0.1 V/s. The developed electrode possesses increased conductance and declined overpotential for the determination of BC. At the optimized conditions, the peak current responses were examined as a function of several variables, including pH, scan rate, the number of deposition cycles, and selectivity. The linear dynamic ranges were found to be 10  $\mu\text{M}$  – 170  $\mu\text{M}$  for BC. The limits of detection (LOD) and quantification (LOQ) were 0.065  $\mu\text{M}$  and 0.21  $\mu\text{M}$ . The PTMCNTPE was successfully applied to determine BC in real samples with percentage recoveries were found to be in the ranges of 95.3 % – 98.5 %.

### **AEP-21: Bifunctional CoFe-LDH/Ni<sub>3</sub>S<sub>2</sub>/NF Electrocatalyst for Efficient Electrocatalytic Water Splitting Coupled with Urea Electrolysis**

**Saad Mehmood, Bapan Biswas and Ujjwal Pal\***

*CSIR-IICT Hyderabad  
E-mail: saadmehmood787@gmail.com, ujjwalpal.iict@nic.in*

In this study, a highly efficient bifunctional electrocatalyst was developed by integrating hydrothermally grown ultrathin cobalt–iron layered double hydroxide (CoFe-LDH) nanosheets with hydrogen

bubble-templated, electrodeposited porous nickel sulfide ( $\text{Ni}_3\text{S}_2$ ) on nickel foam (NF). The resulting CoFe-LDH/ $\text{Ni}_3\text{S}_2$ /NF heterostructure exhibits exceptional catalytic activity and stability toward both hydrogen and oxygen evolution reactions (HER and OER), as well as the urea oxidation reaction (UOR), in alkaline media. Remarkably low overpotentials of  $-60$  mV,  $194$  mV, and  $180$  mV vs. RHE are achieved at a current density of  $10 \text{ mA cm}^{-2}$  for HER, OER, and UOR, respectively. When employed as both the anode and cathode, the CoFe-LDH/ $\text{Ni}_3\text{S}_2$ /NF catalyst drives overall water splitting and urea-assisted electrolysis at cell voltages of only  $1.52$  V and  $1.34$  V, respectively, to deliver  $10 \text{ mA cm}^{-2}$ . Moreover, the system maintains excellent operational stability for 48 hours in overall water splitting and 38 hours in urea electrolysis. These results highlight the synergistic interaction between CoFe-LDH and  $\text{Ni}_3\text{S}_2$ , establishing CoFe-LDH/ $\text{Ni}_3\text{S}_2$ /NF as a promising and durable bifunctional electrode for sustainable hydrogen production and wastewater-assisted energy conversion.

## **AEP-22: Unlocking the Corrosion Inhibition Potential of Expired Chlorzoxazone on Mild Steel in Acidic Media: A Synergistic Approach with Electrochemical, Surface and Computational Insights**

**Jyothi C. Abbar\***

*<sup>†</sup>BMS Institute of Technology and Management, Affiliated to Visvesvaraya Technological University, Bengaluru, Karnataka 560119  
E-mail: jyothiabbar@gmail.com*

With performance evaluated over a temperature range of  $303$  K to  $333$  K, this study investigates the use of the expired drug chlorzoxazone as a mild steel corrosion inhibitor in a  $1.0$  M hydrochloric acid solution. Surface analysis techniques were used in conjunction with weight loss and electrochemical procedures. The addition of inhibitor led to a higher charge transfer resistance at an interface of steel-solution, as revealed by impedance analysis. Potentiodynamic polarization tests demonstrated that the expired CHZ drug markedly reduced the corrosion current density and functioned as a mixed-type corrosion inhibitor, through electrostatic interactions, in line with Langmuir's isotherm model. CHZ demonstrated  $88.3\%$  inhibition at a  $1.0$  ppm inhibitor concentration at  $303$  K. The standard enthalpy of adsorption of  $-10$  kJ/mol indicating CHZ undergoes physical adsorption on MS surface. Additionally,  $E_a^* = 19.4$  kJ/mol observed in the presence of CHZ inhibitor, compared to blank solution, further supports the predominance of physisorption. Surface analysis of inhibited and

uninhibited steel specimens viz. elemental analysis, FT-IR, and AFM, water contact angle measurements were done. Parallel studies were conducted utilizing quantum mechanics-based Density Functional Theory simulations to computationally investigate the system. The overall results shown the corrosion inhibition efficiency of CHZ on steel.

### **AEP-23: Electrochemical Sensing of Perfluorooctanoic Acid (PFOA) Using Hafnium-Doped Tungsten Oxide (Hf-WO<sub>3</sub>) in a Carbon Matrix**

**P.L. Timmanagoudar<sup>1\*</sup>, Madasu Sreenivasulu<sup>2</sup> and Nagaraj P. Shetti<sup>2\*</sup>**

<sup>1</sup>*Department of Chemistry, Basaveshwara Engineering College, Bagalkot-587103, Karnataka*

<sup>2</sup>*Center for Energy and Environment, School of Advanced Sciences, KLE Technological University, Hubballi-580031, Karnataka*  
E-mail: tgoudarprakash@gmail.com; npshetti@kletech.ac.in

Highly toxic perfluorooctanoic acid (PFOA) has been widely employed in the manufacture of household products and is known to pose significant risks to human health and hygiene, leading to extensive environmental contamination, particularly in water and soil. In this study, a hafnium-doped tungsten oxide (HfWO<sub>3</sub>)-modified carbon paste electrode was developed for the first time to enable trace-level determination of PFOA using electrochemical techniques, which offer cost-effective, simple, and selective detection at low concentrations. Hf-WO<sub>3</sub> nanoparticles were synthesised via a hydrothermal route and characterized using XRD, TEM, EDX, and XPS to assess their structural purity and crystallinity. The synthesized nanoparticles were subsequently employed to modify the base electrode. Voltammetric measurements revealed that the Hf-WO<sub>3</sub>/CPE exhibited markedly enhanced sensitivity compared with the unmodified electrode. The influence of electrolyte pH, scan rate, temperature, immersion time, and analyte concentration (linear range:  $7.0 \times 10^{-8}$  M to  $3.0 \times 10^{-4}$  M) was systematically investigated using CV and SWV. Thermodynamic parameters, including enthalpy, entropy, and activation energy, were determined through temperature-dependent studies. The limit of detection (LOD) of the developed electrode was found to be  $1.83 \times 10^{-8}$  M. The practical applicability of the sensor for PFOA determination was evaluated using spiked soil, water, spoiled vegetable, and spoiled fruit samples, yielding %RSD values between 2.88 and 5.94. Interference studies further confirmed the high selectivity of the electrode towards PFOA.

## **AEP-24: Electrochemical Properties of Cobalt Chromite Nanoparticles Synthesized by the Solution Combustion Method**

**Nilesh Chougala<sup>1</sup>, Shidaling Matteppanavar<sup>2</sup>, A. S. Patil<sup>1</sup>  
and V. H. Choudapur<sup>1\*</sup>**

<sup>1</sup>*Department of Physics, KLE Technological University, Hubballi 580031, Karnataka*

<sup>2</sup>*Department of Physics, KLE Society's Basavaprabhu Kore Arts Science and Commerce College, Chikodi 591201, Karnataka*  
*E-mail: veena\_choudapur@kletech.ac.in*

The spherical cobalt chromite nanoparticles were synthesized via solution combustion method. XRD studies confirmed the formation of a cubic spinel  $\text{CoCr}_2\text{O}_4$  structure. Morphological characterization by SEM and TEM revealed highly porous, sphere-like agglomerated nanoparticles. The electrochemical behaviour of the synthesized  $\text{CoCr}_2\text{O}_4$  nanoparticles was evaluated using a stainless-steel (SS) current collector in a 1 M KOH aqueous electrolyte. The  $\text{CoCr}_2\text{O}_4$  exhibited a quasi-rectangular CV profile, indicating a combination of electric double-layer capacitance and pseudocapacitive redox behaviour arising from the  $\text{Co}^{2+}/\text{Co}^{3+}$  and  $\text{Cr}^{3+}$  surface transitions. At a scan rate of  $10 \text{ mV s}^{-1}$ , the electrode delivered a specific capacitance of  $50.6 \text{ F g}^{-1}$ , confirming its ability to store and release charge efficiently. The corresponding energy density was calculated to be  $1.2 \text{ Wh kg}^{-1}$ , which is suitable for low-power energy storage applications. Cycle stability studies further demonstrated that the  $\text{CoCr}_2\text{O}_4$ -modified electrode retains a significant percentage of its initial capacitance over repeated charge-discharge cycles.

## **AEP-25: Sensing of Adenine Using Electrochemical Modified Riboflavin Carbon Paste Sensor for Voltammetric Analysis**

**Kanthappa B. and J.G. Manjunatha\***

*\*Department of Chemistry FMKMC, College, Madikeri, Mangalore University  
Constituent College, Karnataka-571201*  
*E-mail: manju1853@gmail.com*

This work presents an electrochemical method for analyzing adenine (AD) using an electro-polymerized riboflavin-modified graphite paste sensor (PARFMGPS). The sensor was fabricated by depositing a riboflavin polymer film onto the graphite paste surface, enhancing electron transfer and adsorption toward AD oxidation. CV and DPV techniques were used to study AD oxidation behavior and quantify AD under optimized conditions. The modified electrode produced a sharp anodic peak with much higher current than the bare electrode. A

wide linear response range, high sensitivity, and low detection limit confirmed the strong analytical performance. The effects of pH, scan rate (0.025–0.375 V/s), and AD concentration (0.2–200  $\mu$ M for CV and 0.2–270  $\mu$ M for DPV) were evaluated. The riboflavin-modified sensor displayed good repeatability and reproducibility. It also showed excellent stability and resistance to interference. Practical applicability was verified through successful AD detection in biological and pharmaceutical samples. Overall, the method offers a simple, cost-effective, and eco-friendly voltammetric platform for AD determination.

### **AEP-26: A Poly(DL-Phenylalanine) modified Biosynthesized ZnO Nanoparticle Composite Carbon Paste Electrode for the Analysis of Melatonin a Biosensor Study**

**Theertha Thangamma B.S.<sup>1,2</sup>, J G Manjunatha<sup>1\*</sup> and Sumanth D.<sup>1</sup>**

<sup>1</sup>*Department of Chemistry, FMKMC College, Constituent College of Mangalore University, Madikeri 571201, Karnataka*

<sup>2</sup>*Department of Chemistry, Sri Jayachamarajendra College of Engineering, JSS Science and Technology University, Mysuru*  
E-mail: manju1853@gmail.com

A new electrochemical sensor was designed for the accurate and selective analysis of melatonin (ML). The electrode was prepared by modifying a bare carbon paste electrode with biosynthesized Zinc oxide nanoparticles (BZnONP<sub>s</sub>/CPE) and further coated with an electrochemically polymerized DL- phenylalanine (DLP) film (P(DLP)MZnONP<sub>s</sub>/CPE). The polymer layer enhanced the electrode surface and significantly improved the redox response of ML, with the optimum peak obtained in 0.2 M phosphate buffer solution (PBS) at pH 4.0. The surface morphology and elemental composition were examined using scanning electron microscopy (SEM), Energy-Dispersive X-ray Spectroscopy (EDX), and X ray diffraction (XRD). Electrochemical characteristics were explored through cyclic voltammetry (CV), linear sweep voltammetry (LSV), differential pulse voltammetry (DPV), and impedance spectroscopy (EIS). The scan rate results indicated that the oxidation process was diffusion controlled. The modified electrode displayed enhanced current responses across a broad concentration range for both LSV and DPV analyses. The detection limits were calculated as 0.50 $\mu$ M and 0.53 $\mu$ M with corresponding limits of 1.69 $\mu$ M and 1.79 $\mu$ M using LSV and DPV, respectively. The P(DLP)MZnONPs/CPE sensor also exhibited strong tolerance towards interfering metal ions and organic molecules, along with consistent reproducibility, repeatability and stability. Furthermore, it enabled the simultaneous determination of melatonin and adenosine (ADN) and tryptophan (TR).

The applicability of the developed electrode was verified by analysing pharmaceutical tablet samples, where precise and consistent results were obtained.

### **AEP-27: $\text{Sr}_2\text{ZnWO}_6/\text{S-g-C}_3\text{N}_4$ Nanocomposite as a Multifunctional Platform for Pharmaceutical Sensing, Super Capacitive Performance, and Heterocyclic Synthesis.**

**Sanjay. G.S.<sup>1</sup>, Sandeep S.<sup>1\*</sup>, Santhosh A.S.<sup>2</sup> and P.Mallu<sup>1</sup>**

<sup>1</sup>*Department of Chemistry, SJCE, JSS Science and Technology University, Mysuru, Karnataka-570006*

<sup>2</sup>*Department of Chemistry, NMKRV, Jayanagar, Bengaluru, Karnataka-570011*  
E-mail: sanjaygsshaiva2206@gmail.com

An electrochemical sensor was developed for the quantitative determination of chlorambucil (CLB), a chemotherapy drug widely used in cancer treatment. The  $\text{Sr}_2\text{ZnWO}_6$  double perovskite was synthesised via the sol-gel method, and sulphur-doped graphitic carbon nitride (S-GCN) was prepared by thermal polycondensation using urea and thiourea. The  $\text{Sr}_2\text{ZnWO}_6/\text{SGCN}$  nanocomposite was then fabricated through ultrasonic-assisted decoration of  $\text{Sr}_2\text{ZnWO}_6$  onto S-GCN, significantly enhancing sensor performance by amplifying the oxidation signal of CLB. The modified glassy carbon electrode (GCE) exhibited high conductivity, rapid electron transfer, and increased surface reactivity. Electrochemical characterisation techniques such as cyclic voltammetry (CV), linear sweep voltammetry (LSV), and electrochemical impedance spectroscopy (EIS) were employed to evaluate sensor efficacy. Optimised conditions yielded a limit of detection (LOD) of 0.87  $\mu\text{M}$  and a limit of quantification (LOQ) of 2.89  $\mu\text{M}$  with excellent selectivity and stability. The sensor successfully quantified CLB in commercial Leukeran tablets, demonstrating practical pharmaceutical application. Moreover, the  $\text{Sr}_2\text{ZnWO}_6/\text{SGCN}$  nanocomposite exhibited superior electrochemical energy storage capabilities with a specific capacitance of 348.8  $\text{F g}^{-1}$  at 2  $\text{Ag}^{-1}$  and maintained 222.2  $\text{F g}^{-1}$  at 10  $\text{Ag}^{-1}$ , along with a power density of 400  $\text{W kg}^{-1}$  and energy density of 39  $\text{Wh kg}^{-1}$ . Additionally, the material catalysed the green synthesis of benzimidazole derivatives under mild conditions with 95% yield. This multifunctional nanocomposite bridges advanced electrochemical sensing, energy storage, and sustainable catalysis, advancing applications in pharmaceutical analysis and green chemistry.

## **AEP-28: Novel Approach for the Detection of Oxybutynin Hydrochloride using PANI Modified Sensor**

**Sandeep R. Kurundawade, Krishna Naik and Sharanappa T. Nandibewoor\***

*Department of Chemistry, School of Advanced Sciences, KLE Technological University, Hubballi-580031  
E-mail : sandeep@kletech.ac.in*

A novel electrochemical sensor for detecting Oxybutynin Hydrochloride (OBH) was developed using a polyaniline (PANI)-modified Glassy Carbon Electrode (GCE). The PANI modification significantly enhanced OBH's electrochemical response by increasing the electrode's surface area and electrocatalytic properties. The modifier was characterized using X-ray diffraction (XRD) and scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDS). Cyclic voltammetry (CV) and square wave voltammetry (SWV) were employed to investigate OBH's electrochemical behavior. An optimal immersion time of 40 seconds was determined. The study revealed enhanced OBH oxidation at a pH of 7.4 within a potential range of 0.5 V to 1.5 V, indicating an irreversible, diffusion-controlled process. The transfer coefficient ( $\alpha$ ) was 0.51, two electrons ( $n$ ) were involved, and the heterogeneous rate constant ( $k_p$ ) was  $0.58 \text{ ms}^{-1}$ . Under optimized conditions, the oxidation peak current of OBH was linearly proportional to its concentration from  $0.04 \text{ }\mu\text{M}$  to  $10 \text{ }\mu\text{M}$ , with a detection limit ( $D_L$ ) of  $9.16 \text{ nM}$ . This sensor effectively quantified OBH in pharmaceutical samples, demonstrating high recovery, stability, and sensitivity. These results highlight its potential for pharmacokinetic studies and quality control applications, paving the way for further electrochemical exploration of OBH.

## **AEP-29: Voltammetric Analysis of the Synthetic Dye Sunset Yellow at a Poly(asparagine) Modified Chitosan-Capped Silver Nanoparticle/Carbon Nanotube Composite Electrode**

**Sumanth Devaraj and J. G. Manjunatha\***

*\*Department of Chemistry, FMKMC College, Mangalore University Constituent College, Madikeri 571201, Karnataka  
E-mail: manju1853@gmail.com*

This work introduces a simple and effective voltammetric method for detecting the synthetic dye Sunset Yellow (SY) using a newly developed electrode fabricated from poly(asparagine) modified chitosan-capped silver nanoparticles and carbon nanotube composite paste



electrode (P(AS)-Ch@AgNPs/CNTPE). The fabricated sensor's performance was studied using cyclic voltammetry (CV), and linear sweep voltammetry (LSV), which helped understand the redox behaviour of SY and confirm the improved response of the modified electrode. SY gave a clear and well-defined redox signal in phosphate buffer solution (PBS) at pH 6.0, which was selected as the optimal medium for analysis. The surface characterization of both the modified and bare chitosan-capped silver nanoparticles and carbon nanotube composite paste electrode (B-Ch@AgNPs/CNTPE) were studied using SEM, XRD and FTIR techniques to confirm the proper surface coverage and the presence of silver nanoparticles. The scan rate study showed that the electrochemical process was mainly governed by adsorption, indicating strong interaction between SY and the electrode surface. The sensor showed a low detection limit of 0.42  $\mu\text{M}$  and a quantification limit of 1.4  $\mu\text{M}$ , with stable and repeatable results. It was successfully tested in food samples, confirming its usefulness for practical analysis of synthetic dyes.

### **AEP-30: Corrosion Inhibition Study of Mixed-Type Inhibitor on Mild Steel Using HCl Acid Medium**

**Netravati Gayakwad**

*Department of Chemistry, School of Advanced Sciences, KLE Technological University, Vidyanagar, Hubballi -580 031, Karnataka  
E-mail : netravati.gayakwad@kletech.ac.in*

Corrosion, which used to be a problem mainly studied by metallurgists and chemists, is now a topic that involves many different areas of study. This is because metals are used in almost every part of our lives. It's important now more than ever to pay attention to how metals corrode. The use of metals has increased a lot in all areas of technology. New types of strong alloys are being used, and these are often more likely to corrode in certain ways. Most of the chemicals used to stop corrosion are expensive and can be harmful to living things and the environment. That's why it's important to find cheaper and safer alternatives to use as corrosion inhibitors. Using natural substances to stop metal corrosion in acidic or basic conditions is a new trend. Inhibitors are crucial in slowing down the process of corrosion. There are many different types of inhibitors, including organic ones, which often contain nitrogen, oxygen, and phosphorus. Inorganic inhibitors form protective layers on the metal surface. Plant-based inhibitors, which are biodegradable, contain chemicals from plants that help slow down corrosion. These inhibitors work by slowing down either the anodic or cathodic reactions, or both. This study focuses on mixing organic, plant-based, and inorganic substances to



control corrosion on mild steel in a 0.5M HCl solution. The weight loss method showed 89.39% inhibition for 4 ml, 70.06% for Tafel, and 79.75% for impedance for 4 ml at room temperature.

### **AEP-31: Investigation of Ionizing Radiation Attenuation of Selected Immunotherapy Drugs**

**G.B. Hiremath<sup>1</sup>, V.P. Singh<sup>2</sup>, N.H. Ayachit<sup>1</sup> and N.M. Badiger<sup>1\*</sup>**

<sup>a</sup>*School of Advanced Sciences, KLE Technological University, Hubballi-580031*

<sup>b</sup>*Department of Physics, Karnatak University, Dharwad-580008*

*E-mail : nagappa.badiger@kletech.ac.in; gbhiremath@kletech.ac.in*

The promising results are observed for cancer treatment when immunotherapy is combined with radiation therapy, and it is useful to examine radiation interaction with immunotherapy drugs. In this view, the radiation interaction and dosimetric parameters of selected immunotherapy drugs such as avelumab, bevacizumab, durvalumab, and trastuzumab were studied using EpiXs software and PSTAR database. The mass attenuation and energy absorption coefficients of selected immunotherapy drugs are indistinguishable. Variation in the  $Z_{\text{eff}}$  lies in the energy range from 3 to 10 keV. The total stopping power of protons was estimated using the PSTAR database, and it was found that Bragg's peak is around 0.06 MeV for all selected immunotherapy drugs. This study will be helpful in many research areas, such as medical applications, radiation protection, and radiation chemistry.

### **AEP-32: A Novel Voltammetric Method for the Enhanced Detection of the Food Additive Vanillin Using an Electrochemical Sensor**

**B.M. Amrutha and J.G. Manjunatha\***

*Department of Chemistry, FMKMC College, Constituent College of Mangalore University, Madikeri, Karnataka*

*E-mail : manju1853@gmail.com*

Vanillin (VN) is a primary constituent of Vanilla which is a commonly used flavouring agent in the food and pharmaceutical industry. Electrochemical property of VN and Caffeine (CF) at Poly Alanic acid modified carbon nano tube paste electrode (PAMCNTPE) was examined by cyclic voltammetry (CV) and differential pulse voltammetry (DPV) in 0.2 M phosphate buffer solution (PBS) of an optimum pH of 6.5. Field emission scanning electron microscopy (FE-SEM) was used to compare the surface morphology of PAMCNTPE and a bare carbon nano tube paste electrode (BCNTPE), and electrochemical impedance spectroscopy was used to analyse the kinetics of electron transport (EIS). The increased surface area and

interactions between the polymer film and analyte are responsible for PAMCNTPE's superior electrocatalytic activity for the oxidation of VN. The VN sensor showed a low detection limit of 0.17 M by the DPV method. In spite of prominent interferents as metal ions and organic species, the constructed sensor's selectivity for VN detection was impressive. This facile VN sensor can be effectively used for real sample analysis, due to its simplicity and stability.

## INORGANIC CHEMISTRY SECTION

### Sectional President's Address

#### Synthesis and Spectroscopic Studies on Some Transition Metal Complexes with Acyclic and Macrocyclic Ligands

V. K. Sharma

*Department of Chemistry, University of Lucknow, Lucknow-226007  
E-mail: vksharma21@hotmail.com; sharma\_vk@lkouniv.ac.in*

The field of coordination chemistry of acyclic and macrocyclic compounds has undergone spectacular growth during last four decades. This growth has largely been due to the synthesis of a great number and variety of coordinating ligands for metal ions. This remarkable progress in the field of metal complexes may be attributed to their diversified applications. These complexes have been finding use in the field of homogeneous catalysis, various biological systems, potential drugs and analytical chemistry. On account of their wider applicability, metal complexes of transition series, lanthanides, actinides, alkali and alkaline earth metals have been studied with donors such as nitrogen, oxygen, sulphur and halogens. Cr(III), Mn(III), Fe(III) and Co(III) complexes of thiosemicarbazones, derived from benzil á-monoxime and thiosemicarbazides (BMTH<sub>2</sub>), benzil á-monoxime and phenyl thiosemicarbazides (BMPH<sub>2</sub>), benzil á-monoxime and 4-bromophenyl thiosemicarbazides (BMBH<sub>2</sub>), benzil á-monoxime and 4-chlorophenyl thiosemicarbazides (BMCH<sub>2</sub>) and benzil á-monoxime and 4-nitrophenyl thiosemicarbazides (BMNH<sub>2</sub>), have been prepared. These complexes have been characterized by elemental analyses, magnetic susceptibilities, molar conductance measurements, electronic, IR, <sup>1</sup>H and <sup>13</sup>C NMR spectra (in the case of Co(III) complexes), FAB mass and thermogravimetric analysis to arrive at the geometry of the ligand environment around the metal ion and to elucidate the bonding sites of the ligands with the central metal ion. The complexes contain two monoprotonic tridentate ligands with NNS donor sites. Coordination to central metal ion via the oxime nitrogen, imine nitrogen and thione sulphur is confirmed in the complexes via i.r. spectral studies. The antifungal and antibacterial activities of the ligands and its complexes have been screened.

## **IIL-01: Synthetic Metal-chelates in Medicines: Possibilities and Prospects**

**A.P. Mishra**

*Department of Chemistry, Dr. H. S. Gour Vishwavidyalaya (Central University), Sagar-470003*

*E-mail: apmishrasagar@gmail.com*

The Pandemic Covid-19, forced medicinal scientists to view and review the chemotherapeutic search including use of Purposed and Re-purposed drugs. Can metallodrugs or metal-chelates, be an Alternative or Supplementary medicines? The Challenges and Possibilities, are before us to answer by making intensive researches. The interfacial studies overlapping Inorganic chemistry and Biomedical sciences, have attracted the attention of bioinorganic scientists in search of novel pharmacophores and metallodrugs. There are several references in indigenous Indian medicinal system Ayurveda, on metallothrapy/ Rasayan. The contribution of Ehrlich (1909), a Nobel Laureate in form of a metallodrug Arsenic-amine (Salvarsan), has significantly been highlighted, as father of chemotherapy in modern medicinal practices. However, medicinal inorganic chemistry remains an underestimated area within medicinal chemistry and the main reason is the mislead association of metals to toxic agents, though metal-chelates of life-essential metal ions are atleast harmful (in comparison to antibiotics), if taken as per doses @ RDA.

The metal complexes are amenable to combinatorial synthetic methods and an immense diversity of structural scaffolds can be achieved. Metal centers are capable of organizing surrounding molecules to achieve pharmacophoric geometries that are not readily achieved by other means. Understanding these interactions can lead the way towards rational design of metallopharmaceuticals implementations of new co-therapies. The design and synthesis of a suitable ligand, perhaps is the key step in the development of coordination complexes with unique properties and novel reactivity. Synergistically tailored and monitored Chelation Therapy approach, can minimize and nullify the metal toxication issues. Principle of Reverse Pharmacology may help substantially in restoring the concept and therapeutic use practices of Traditional Medicinal systems, on issues to prevent and minimize the prevalent attacks of mutating and resisting microbes including viruses and fungi.

Metal complexes derived from Schiff bases and its derivatives have been studied extensively due to their facile synthesis, unusual configurations, and structural labiality. The insertion of designed Schiff bases as ligands in metal coordination sphere produces specific

functionalities and exciting features with interesting theoretical and practical applications. Related issues shall be discussed in this lecture.

### **IIL-02: Functional Materials of Thioate and Phosphoro-thioates Metal Complexes**

**Umesh Nath Tripathi**

*Professor, Department of Chemistry, D. D. U. Gorakhpur University,  
Gorakhpur-273009*

*E-mail : un\_tripathi@yahoo.com*

Chelating ligands containing thioate sulfur donors have played a pivotal role in coordination chemistry for over a century. Representative systems such as dithiocarbamates, xanthates, and di- or trithiocarbonates are known for their biological significance and diverse practical applications. Incorporating phosphorus adjacent to sulfur in the ligand framework as in dithiophosphate and trithiophosphate derivatives significantly improves electron-donating capacity and introduces versatile coordination modes. This structural modification facilitates the formation of stable and reactive assemblies with tailored electronic properties. Such multifunctional ligands have proven valuable in designing highly selective catalysts, developing molecular electronic materials, and constructing biomimetic complexes that model enzymatic active sites.

Metal–thioate complexes, in particular, constitute a versatile class of materials characterized by diverse bonding modes, chemical robustness, and wide applicability in catalysis, electronic devices, and biological systems. The strong affinity of sulfur for transition metals enables the construction of complexes with tunable geometries and functionalities, where thioate ligands can act as mono-, bi-, or polydentate donors or as bridges in multinuclear frameworks. Continued progress in the synthesis and structural modulation of phosphorus–thioate complexes is expanding their potential in materials science, offering new opportunities for sustainable catalysis and optoelectronic technologies.

### **IIL-03: Cu(II)-DEAS Functionalized MIL-101(Cr)-NH<sub>2</sub> : A Robust MOF-Based Catalyst for Efficient Synthesis of 3,5-Disubstituted-1,2,4-Triazoles**

**Pritish Rajkumar Moon, Jyoti Prabha Kujur and  
Devendra Deo Pathak\***

*Department of Chemistry and Chemical Biology, Indian Institute of  
Technology (ISM), Dhanbad-826004*

*\*E-mail : ddpathak@iitism.ac.in*

The 2025 Nobel Prize in Chemistry has witnessed the emerging

significance of Metal Organic Frameworks (MOFs) in gas storage and separation, catalysis, chemical sensing, and drug delivery. MOFs have proved to be versatile platforms in heterogeneous catalysis due to their exceptional porosity, large surface area, high thermal stability, tunable surface functionality, unique geometric/electronic configurations, etc. Surprisingly, approximately 80–90% of industrial chemical processes rely on heterogeneous catalysis. Prompted by these results, the synthesis of a MOF-based catalyst, MIL-101(Cr)@DEAS-Cu(II), is carried out and its application, as an efficient heterogeneous catalyst, is demonstrated in the one-pot synthesis of a series of pharmaceutically active 3,5-disubstituted-1,2,4-triazoles from benzylamines and benzonitriles under solvent-, base- and additive-free conditions. During the presentation, synthetic details and characterization of MOF supported complex DEAS-Cu(II) by various physicochemical methods (FT-IR, XRD, XPS, SEM, TEM, EDX, TGA, BET, and ICP analyses) will be unravelled along with the Green Chemistry metrics such as AE, E-factor, CE, PMI, and RME. The obvious advantages of this catalyst over the homogeneous counterpart will be disclosed.

#### **IIL-04: $\text{MgFe}_2\text{O}_4\text{@SiO}_2\text{-SO}_3\text{H}$ : as A Novel Heterogeneous Magnetic Nanocatalyst for the Synthesis of Benzoxazinone and Benzthioxazinone via Multicomponent Reactions under Solvent Free Conditions**

**A. S. Aswar**

*Department of Chemistry, Sant Gadge Baba Amravati University,  
Amravati - 444602  
E-mail : aswaranand@gmail.com*

Catalysis is a very rewarding field and magnetic recovery of catalyst added a further greener approach to it. In the context of Green Chemistry catalysis has received a remarkable interest, both from a scientific and an industrial perspective. During the recent year's silica-coated magnetic nanoparticles have been found very useful and interesting applications due to its unique characteristics which make it suitable for different applications. The surface functionalization of silica-coated magnetic nanoparticles using reactive organic and inorganic group allows synthesis of multifunctional of silica-coated magnetic nanoparticles. Moreover, structural, magnetic and optical environments in spinel ferrites can be quite different, due to the distribution of iron and the divalent metal ions among the tetrahedral and octahedral sites of the spinel lattice. Recently, we have developed a number heterogeneous supported catalysts which showed improved

efficiency for several important organic transformations. In the present work, we have reported the synthesis and characterization of  $\text{MgFe}_2\text{O}_4@\text{SiO}_2-\text{SO}_3\text{H}$  as a novel and green nanomagnetic solid acid catalyst, which is containing the sulfuric acid catalytic sites on the surface of  $\text{MgFe}_2\text{O}_4$  magnetic nanoparticles as the catalytic support. The characterization of catalyst was made by XRD, FT-IR, TGA, SEM-EDS, TEM and surface area measurements. The performance catalyst towards different multicomponent reactions such as benzoxazinones, benzthioxazinones, imidazole, pyranopyrazoles etc. have been explored under solvent free conditions. Furthermore, the activity of the recycled nanocatalyst least was also examined for at least five cycles with a negligible loss of its activity. The product distribution pattern with the variation of different reaction conditions such as reaction temperature, solvent, molar ratio, effect of energy source, concentration of catalyst and reaction time. The attractive features of this protocol are its greenness with respect to mild reaction conditions, high activity, and easy work-up, excellent yield and reusability of a catalyst. All synthesized compounds were characterized by various physiochemical techniques such as  $^1\text{H}$  &  $^{13}\text{C}$ -NMR, FTIR, Mass spectral data, melting points and compared with literature values.

### **III-05: Synthesized Carbon Dot as Excellent Corrosion Inhibitor for Mild Steel in HCl Solution**

**M. Yadav\* and Pooja Kumari**

*Department of Chemistry and Chemical Biology, IIT(ISM), Dhanbad-826004  
E-mail : mahendra@iitism.ac.in*

Heteroatom-doped Carbon dots (CDs) have been recognized as efficient eco-friendly corrosion inhibitors due to their low cost, excellent chemical stability, good water solubility, and nontoxic properties. In the present investigation a nitrogen-doped eco-friendly carbon dot was synthesized using a one-step hydrothermal process, and its corrosion inhibition performance for the mild steel (MS) in 15% HCl solution was studied. The synthesized carbon dot was characterised by Fourier transform infrared (FTIR), X-ray photoelectron spectroscopy (XPS), ultraviolet-visible spectroscopy, photoluminescence (PL), and high-resolution transmission electron microscopy (HRTEM). The corrosion inhibition efficiency of the synthesized carbon dot was studied using weight-loss, electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization studies. Corrosion inhibition efficiency of inhibitor increases with increasing concentration and reaching 96.8% after 6 h immersion at 150 ppm concentration. The adsorption of inhibitor on MS obeyed Langmuir adsorption isotherm and physical adsorption process. Potentiodynamic polarization study suggested that



this inhibitor acts as mixed type inhibitor and alter the rates of anodic dissolution of MS and cathodic hydrogen evolution reaction simultaneously. The field emission scanning electron microscopy (FESEM) and atomic force microscopy (AFM) and XPS studies confirmed the formation of protective film of inhibitor molecules at the MS surface.

### **III-06: Low Cost Electrocatalysts for Sustainable Green Hydrogen Production**

**T. Maiyalagan\***

*Electrochemical Energy Laboratory, Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur - 603203*  
*E-mail : maiyalagan@gmail.com*

Electrochemical water splitting has emerged as a highly promising approach for clean and large- scale hydrogen generation, offering a pathway toward zero-carbon energy systems. Despite its potential, practical implementation is still restricted by slow reaction kinetics and the heavy reliance on precious-metal catalysts. To overcome these limitations, significant research efforts have centered on creating cost-effective, efficient, and durable electrocatalysts for both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). In our work, we have developed a series of noble-metal-free materials that demonstrate remarkable catalytic activity for HER, OER, and overall water splitting. An ideal electrocatalyst must simultaneously provide:

(1) intrinsically active catalytic sites, (2) large accessible surface area, (3) rapid electron and mass transport pathways, (4) strong chemical and structural robustness, and (5) low-cost, scalable synthetic routes. Although progress has been substantial, many existing studies focus on only a subset of these requirements, often emphasizing electronic tuning of active sites. This presentation will highlight recent progress in the development of noble-metal-free HER catalysts, with particular emphasis on molybdenum-based systems such as  $\text{MoO}_2$ ,  $\text{Mo}_2\text{S}$  and  $\text{Mo}_2\text{C}$ . These earth-abundant materials have attracted great interest due to their high HER activity, tunable electronic properties, and cost-effectiveness. I will also discuss advanced strategies that further enhance their performance and durability, including the formation of Mo-based carbon composites, heteroatom doping for electronic modulation, and the construction of heterostructures that enable synergistic catalytic effects. Finally, I will address the remaining challenges and potential future directions in the field of Mo-based electrocatalysts, with the broader goal of advancing scalable and sustainable hydrogen-production technologies.

### **IIL-07: Role of In Situ Generated Organometallic Complexes in the Construction and Functionalization of Late-Stage Heterocycles**

**Neeraj Kumar Mishra**

*Department of Chemistry, Faculty of Science, University of Lucknow,  
Lucknow - 226007, U.P.*

*E-mail: neerajchemistry@gmail.com*

With the significant progress in the construction of late-stage drug candidates, in situ generated organometallic complexes deliver an important platform. Directly in the reaction mixture, in situ formation of reactive metal-complexes offers a greater control, broader functional group compatibility, and access to unique reactivities that bypass the challenges associated with using preformed, highly sensitive reagents. Using organometallic complexes generated directly during the reactions has various benefits such as enhanced control, mild conditions, operational simplicity, and strategic flexibility. In situ organometallic complexes enables the C–H activation and functionalization and are central to cross-coupling reactions, which forms C–C and C–heteroatom bonds of various drug molecules. In situ monitoring techniques, like real-time spectroscopy, are also key to understanding the formation and role of these transient complexes, which is crucial for optimizing reactions for complex late-stage heterocycles. Therefore, the design, and in situ generation of organometallic complexes is highly attractive in functional materials, pharmaceutical and agrochemicals industries. In this context, from last few years, our groups reported a range of in situ generated organometallic complexes for the late-stage heterocycles formation and functionalization via C–H bond activation with the help of various directing groups.

Herein, during my presentation, I will describe a brief summary of our recent works and present progress works on the role and utility of in situ generated organometallic complexes to synthesize the late-stage biologically relevant heterocyclic drug candidates.

### **IIL-08: Metal-Organic Frameworks: Nobel-Worthy Materials Shaping Modern Chemistry**

**M. Rajeswara Rao**

*Department of Chemistry, Indian Institute of Technology, Dharwad - 580011  
E-mail: rajesh@iitdh.ac.in*

Metal–organic frameworks (MOFs) are crystalline porous materials constructed from metal ions or clusters linked by organic ligands, forming highly ordered, tunable three-dimensional networks. They exhibit exceptional properties such as ultra-high surface area, permanent porosity, and customizable chemical functionality. These

features enable applications in gas storage, CO<sub>2</sub> capture, catalysis, drug delivery, sensing, and separation processes.

MOFs exemplify the broader principles of metal-organic chemistry, which studies metal–ligand bonding and reactivity. Advances in ligand design allow precise control over electronic and steric environments around metal centres. Such control enhances stability and selectivity in both molecular catalysts and extended frameworks. In my talk, I will highlight the design, synthesis and applications of MOFs and how these materials will shape the future of the world.

### **IO-01: Synthesis and Characterization of Dysprosium(III) Complexes with Dimethylmalonate and N, N'-donor auxiliary Ligands for Advanced Luminescent Materials**

**Ritu Langyan\* and Shagun Chaudhary**

*Department of Chemistry, Kurukshetra University, Kurukshetra-136119, Haryana  
E-mail : ritu.langyan@gmail.com*

Dysprosium(III) complexes have emerged as highly promising luminescent materials due to their sharp blue-yellow emissions originating from 4f–4f electronic transitions. However, the inherently weak Laporte-forbidden transitions in Dy(III) ions restrict their direct excitation efficiency. To address this, a series of Dy(III) complexes was synthesized using a ligand, dimethylmalonate, as the primary sensitizer, combined with N, N'-donor auxiliary ligands including 2,2'-bipyridine and 4-methyl-1,10-phenanthroline to enhance luminescence via the antenna effect. These ligands engage in strong light absorption with  $\pi\text{--}\pi^*$  transitions, facilitating efficient intramolecular energy transfer to the Dy(III) ion's emissive states. Comprehensive characterization through FTIR spectroscopy, elemental analysis, and UV–Vis absorption confirmed successful complex formation and ligand coordination. Photoluminescence investigations revealed distinct spectral features attributed to Dy(III) emissions at 481 nm and 572 nm, corresponding to  $^4\text{F}_{9/2} \rightarrow ^6\text{H}_{15/2}$  and  $^4\text{F}_{9/2} \rightarrow ^6\text{H}_{13/2}$  transitions, respectively. Notably, auxiliary ligands were found to significantly enhance emission intensity and stabilize the complexes. Thermal analyses (TGA/DTA) demonstrated stability more than 200 °C. Furthermore, CIE chromaticity coordinates verified emission within the blue-yellow region, confirming the suitability of these complexes for white light LEDs, display screens, and sensing applications.

## **IO-02: A Rapid Synthesis of Quinoxalines by Using $\text{Al}_2\text{O}_3\text{-ZrO}_2$ as Heterogeneous Catalyst**

**Asmita A. Chandanshive, Premkumar B. Thombre, Sonali A. Korde, Sudarshan S. Dipake, Anjali S. Rajbhoj, Machhindra K. Lande and Suresh T. Gaikwad\***

*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar - 431004 (M.S.)  
E-mail : asmitachandanshive111@gmail.com*

In this study, we present a highly efficient and environmentally benign protocol for synthesizing biologically important Quinoxaline derivatives. The synthesis involves the reaction of 1,2-diamines with substituted phenacyl bromides or benzil, taking place at room temperature in N,N-dimethylformamide (DMF) solvent. The reaction is facilitated by a bifunctional heterogeneous catalyst composed of  $\text{Al}_2\text{O}_3\text{-ZrO}_2$  binary metal oxide. Our method offers numerous advantages, including excellent product yield, renewable catalytic conditions, minimal catalyst usage, safer chemistry, short reaction time and a simple work-up procedure. To determine the chemical structure of the synthesized derivatives, we employed characterization techniques such as Nuclear Magnetic Resonance (NMR) and High-Resolution Mass Spectrometry (HRMS). Additionally, the  $\text{Al}_2\text{O}_3\text{-ZrO}_2$  catalyst was characterized using X-ray Diffraction (XRD), Scanning Electron Microscopy with Energy-Dispersive X-ray Analysis (SEM-EDAX), and Thermogravimetric Analysis (TGA).

## **IO-03: Synthesis, Characterization, Electrochemical Studies, Dye Degradation, Fluorescence, Antioxidant, and Antimicrobial Activities of Novel Bioactive Homo-Binuclear Co(II), Ni(II), Cu(II), and Zn(II) Complexes Derived from an $\text{N}_2\text{O}_2$ -Type Tetradentate Schiff Base Ligand**

**Deepshikha Gupta and A. P. Mishra\***

*Department of Chemistry, Dr. Harisingh Gour Vishwavidyalaya (A Central University), Sagar - 470003, Madhya Pradesh  
E-mail: Deepshikhagupta29@gmail.com; apmishrasagar@gmail.com*

The present study focuses on the synthesis and structural characterization of novel homo-binuclear Co(II), Ni(II), Cu(II), and Zn(II) complexes derived from an  $\text{N}_2\text{O}_2$ -type tetradentate Schiff base ligand. This ligand was synthesized via a condensation reaction between terephthalaldehyde and 2-amino-5-chloro-3-nitrophenol in a 1:2 molar ratio using methanol as the solvent. The resulting compounds were characterized through various techniques including elemental analysis, molar conductance measurements, UV-Vis spectroscopy, FT-IR,  $^1\text{H}$ -NMR,  $^{13}\text{C}$ -NMR, mass spectrometry, and powder X-ray diffraction (XRD).

Thermal stability was evaluated using thermogravimetric and differential thermal analysis (TGA-DTA). Electrochemical properties were investigated using cyclic voltammetry, revealing redox processes related to the coordination environments of the metal centres. Additionally, the complexes were tested for their ability to degrade methylene blue dye. Antibacterial activity was evaluated using the well-diffusion method against *Escherichia coli*, *Pseudomonas aeruginosa*, and *Klebsiella pneumoniae*. Antifungal activity of both the ligand and metal complexes was assessed using the growth inhibition method. Antioxidant activity was examined through the DPPH assay, where the complexes demonstrated notable activity comparable to standard ascorbic acid. Solid-state fluorescence studies were also conducted on the synthesized compounds. These homobinuclear metal complexes show significant activities as advanced functional materials for potential applications in catalysis and biology.

### **IO-04: A Catalytic Activity of Terbium Rare Metal Complex of Quinoline Derivative**

**H. D. Chaudhari**

*Department of Chemistry, Hemchandracharya North Gujarat University, Patan  
E-mail : haresh09032007@gmail.com*

The coordination chemistry of rare-earth metal ions with quinoline-based ligands has garnered increasing attention due to their biological significance and catalytic versatility. Here, we report the synthesis of novel coordination complexes derived from a scarcely investigated quinoline derivative and selected rare-metal perchlorates. The complexes were rigorously characterized through a suite of state-of-the-art spectroscopic and analytical methods, enabling precise structural and physicochemical elucidation. Their catalytic potential was systematically probed under both homogeneous and heterogeneous regimes, while antimicrobial activity was evaluated using standardized biological assays. Importantly, structure–property correlations were established, revealing critical insights into how subtle variations in molecular architecture govern chemical reactivity and biological response. These findings not only broaden the understanding of quinoline–rare metal interactions but also highlight their potential utility in catalysis and therapeutic applications.

### **IO-05: A New, Eco-Friendly and Cost-Effective Method was Developed to Prepare Alumina-Supported 10-molybdo-2-tungstosilicic acid ( $\text{H}_4\text{SiMo}_{10}\text{W}_2\text{O}_{40}/\text{Al}_2\text{O}_3$ ) Catalysts**

**Shital B. Sukale and Sunil G. Shankarwar\***

*Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajanagar  
- 431004, Maharashtra*

*E-mail: shitalsukale11@gmail.com*

These solid acid catalysts were used to efficiently synthesize 2,3-dihydroquinazolin-4(1H)-one derivatives. Their structure and surface properties were analysed using techniques like FT-IR, XRD, BET, FE-SEM, HR-TEM, EDX, and TG-DTA. Among various formulations, the catalyst containing 20%  $\text{H}_4\text{SiMo}_{10}\text{W}_2\text{O}_{40}/\text{Al}_2\text{O}_3$  on alumina showed the highest activity in promoting the reaction between 2-aminobenzamide and aromatic aldehydes. This catalyst is not only highly effective but also reusable without losing its performance. The process offers several benefits including high product yields, mild reaction conditions, short reaction times, non-toxic materials, affordability, and easy product isolation.

### **IO-06: Acid-Catalyzed Dehydrative Imination of Benzil using 2-Amino-4-chloro-5-nitrophenol: Metal Complexation and Their Biological-Environmental-Agricultural Applications**

**Shivanshu Brahmchari and A.P. Mishra\***

*Department of Chemistry, Dr. Harisingh Gour Vishwavidyalaya (A Central University), Sagar - 470003, Madhya Pradesh*

*E-mail: bshivanshu99@gmail.com; apmishrasagar@gmail.com*

The work reports the acid-catalyzed synthesis of a novel benzil-derived Schiff base ligand, 6,6'-((1,2-Diphenylethane-1,2-diylidene)bis(azaneylylidene))bis(4-chloro-3-nitrophenol) (SBE), and its complexes with Co(II), Ni(II), Cu(II), and Zn(II). The ligand was obtained via reflux-assisted condensation of Benzil with 2-Amino-4-chloro-5-nitrophenol. Structural and electronic features were elucidated by UV-Vis, FT-IR,  $^1\text{H}$ -NMR, mass spectrometry, P-XRD, TGA, and supported by DFT studies. Complexation induced distinct spectral shifts and improved thermal stability, confirming metal-ligand coordination through azomethine and phenolic sites. Biological and environmental evaluations revealed diverse activities: fungicidal efficiency of the ligand, strong antioxidant (SBEZn), notable dye degradation (SBECu), and seed germination promotion (SBECu). These findings highlight the multifunctional potential of benzil-based Schiff bases and their

metal complexes as candidates for sustainable biological and environmental applications.

### **IO-07: Organotin(IV) Dithiolate Complexes of 2-Methoxyphenylacetonitrile: Synthesis, Characterization and Cytotoxic Properties**

**Kiran Gupta and Om Prakash\***

*Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow-226007, U.P.*

*E-mail : prakash\_om@lkouniv.ac.in; ops92002@gmail.com*

Three new tetra-coordinated organotin(IV) complexes bearing a dinegative dithiolate derived from 2-methoxy-phenylacetonitrile (2MeO-PAN) were synthesized and formulated as  $[\text{Sn}(\text{OCH}_3\text{PhC}(\text{CN})=\text{CS}_2)(\text{R})_2]$  where  $\text{R}=\text{CH}_3$  (1),  $\text{R}=\text{n-butyl}$  (2), and  $\text{R}=\text{Ph}$  (3). The complexes were characterized by FT-IR,  $^1\text{H}/^{13}\text{C}$  NMR,  $^{119}\text{Sn}$  NMR, UV-Vis, and ESI-MS, supporting  $\kappa^2$  (S, S) chelation of the dithiolate to Sn (IV) in a four-coordinate environment. In vitro cytotoxicity was evaluated over appropriate concentration ranges. The complex (3) exhibited the highest potency with  $\text{IC}_{50} = 15 \mu\text{M}$ , followed by the (1) analogue  $\text{IC}_{50} = 30 \mu\text{M}$ , while the complex (2) was less active ( $\text{IC}_{50} = 50 \mu\text{M}$ ). Consistently, the percent cell death at equipotent levels was ~50–51% for all three systems. These results indicate that aryl substitution at tin enhances anticancer activity relative to alkyl substitution within this ligand framework, potentially reflecting differences in lipophilicity, Sn–C bond polarization, and cellular uptake. The comprehensive spectroscopic suite corroborates the proposed formulations and donor set, while the biological data identify complex (1) as the most promising lead for further mechanistic and structure–activity relationship studies. Overall, this work expands methoxy-benzyl-cyanide-derived dithiolate organotin chemistry and highlights substituent-dependent cytotoxic profiles relevant to organotin-based anticancer agent development.

### **IO-08: Synthesis and Spectral Characterization of Chromium(III) & Iron(III) Complexes with N, O Donor Oxime Ligands**

**Shruti Mishra and V. K. Sharma\***

*Department of Chemistry, University of Lucknow, Lucknow-226007 (U.P.)*

*E-mail : vksharma21@hotmail.com; shruti.dixit7@gmail.com*

Oxime ligands, containing  $-\text{C}=\text{NOH}$  functional group, exhibit strong chelating ability toward transition metal ions through coordination via the azomethine nitrogen and oxime oxygen. Deprotonation enhances their donor strength, enabling the formation of stable chelate rings. Structural features such as syn–anti isomerism and hydrogen



bonding influence their geometry and coordination behaviour. Due to their stability and versatile binding modes, oxime-based metal complexes demonstrate significant potential in analytical, catalytic, and biological applications. A new series of transition metal complexes of Chromium(III) and Iron(III) derivatives have been isolated from different N-substituted isatin-3-oxime ligands. The synthesized complexes were distinguished through physical investigations along with spectral investigation (UV-Vis, IR and  $^1\text{H}$  NMR). The obtained input illustrates that these complexes have octahedral geometry around centre metal ion with N/ O donor atoms. In addition, biological studies and molecular docking have been carried out for investigated compounds.

### **IO-09: Bimetallic Co/Mg Metal-Organic Frameworks for the Adsorptive Removal of Brilliant Green from Aqueous Solutions**

**M.P. Lekha and S. Jitendra Pal\***

*Environmental Remediation Research Lab, Department of Chemical Engineering,  
National Institute of Technology, Surathkal, Mangalore - 575025, Karnataka  
E-mail : lekha.237ch001@nitk.edu.in*

The increasing discharge of synthetic dyes into aquatic ecosystems poses significant threats to ecological balance and biodiversity, necessitating effective remediation strategies to mitigate their toxic impacts. This study aims to develop an efficient adsorbent using Co/Mg bimetallic organic frameworks synthesized via the solvothermal and sonochemical synthesis methods for the removal of brilliant green dye from aqueous solutions. Characterization of the material was conducted using XRD, SEM, BET, FTIR, EDX, and TGA to confirm its structural, morphological, and surface properties. The adsorption studies conducted using brilliant green as a model pollutant to evaluate the dye removal efficiency of the synthesized material under varying experimental conditions have shown an exceptional removal efficiency. These investigations provided insights into the adsorption capacity, kinetics, and reusability of Co/Mg bimetallic organic framework adsorbents, offering a promising pathway toward sustainable and scalable wastewater treatment solutions.

## **IO-10: Studies on the Synthesis, Characterization and Cytotoxicity of Some Transition Metal Complexes of 4-chloro-N'-[(E)-(2-hydroxy-4-methoxyphenyl) Methylidene] Benzohydrazide**

**Kirti Patil and Shashikant D. Ajagekar\***

*Department of Chemistry, Thakur College of Science and Commerce  
(Autonomous), Kandivali (East), Mumbai-400101, Maharashtra  
E-mail : drsdajagekartcsc@gmail.com*

The Schiff base 4-chloro-N'-[(E)-(2-hydroxy-4-methoxyphenyl) methylidene]benzohydrazide (HCBHV), was prepared by using 2-Hydroxy-4-methoxybenzaldehyde (vanillin) and 4-chlorobenzohydrazide. The solid complexes of Cu(II) and Ni(II) were synthesized. Molar conductivity, magnetic susceptibility, X-ray diffraction, Fourier transform infrared, nuclear magnetic resonance, ultraviolet-visible, and mass spectrometry were used to characterize these metal complexes. The metal: ligand ratio in these metal complexes was found to be 1:2 by analyses. The physicochemical investigation provides evidence for the presence of tetrahedral geometry around Cu(II) and octahedral geometry around Ni(II) ions. The IR spectral data shows that the ligand acts as a tridentate with an OON-donor atom sequence towards the central metal ion. Metal complexes are likely non-electrolytes because of their low molar conductance values. X-ray diffraction analyses indicates that these compounds likely adopt a monoclinic crystal structure. *S. aureus* MCC 2408, *B. subtilis* MCC 2010, *P. aeruginosa* MCC 2080, and *E. coli* MCC 2412 were used as test organisms for the HCBHV ligand and their metal complexes for antibacterial and fungicidal activities.

## **IO-11: Transition Metal Complexes Tethered with Water Soluble Schiff bases Derived from Azo Aldehyde and Amino Acids: Synthesis, Characterization and Solution Studies**

**Manasa P. Gunaga and Manasa Kongot\***

*Department of Science and Humanities, Manipal Institute of Technology,  
Bengaluru, Manipal Academy of Higher Education, Manipal  
E-mail : k.manasa@manipal.edu*

Synthesized a series of 3d transition metal complexes by reacting equimolar amounts of water-soluble Schiff base ligands with corresponding metal salts in aqueous–alcoholic media under reflux conditions. The Schiff base ligands were derived from sulfo-azo aldehydes and amino acids, providing versatile donor sites for stable coordination. The resulting colored complexes were isolated in good

yield and characterized using FT-IR and UV-Vis spectroscopy. FT-IR spectra showed characteristic shifts in the azomethine (C=N) and phenolic (C-O) stretching frequencies, confirming coordination through nitrogen and oxygen donor atoms. UV-Vis spectra displayed well-defined d-d transitions, indicating the formation of stable metal-ligand complexes. Solution behavior was further examined through pH-dependent UV-Vis studies to understand the stability and coordination environment of the complexes in aqueous media. Systematic spectral changes with varying pH revealed stepwise metal-ligand interactions and stable complex formation over a broad pH range. These findings demonstrate the adaptability of sulfo-azo Schiff base frameworks toward transition metal complexation and highlight the usefulness of UV-Vis and pH studies in probing their solution properties. Such systems provide a basis for future investigations on their physicochemical behavior and potential applications.

## **IO-12: Design, Spectroscopic Analysis, and Molecular Docking of S-Benzyl $\beta$ -(N-3,5-dichloro-2-hydroxybenzylidene) dithiocarbazate as a Potential SARS-CoV-2 Main Protease Inhibitor**

**Rayees A. Bhat<sup>1\*</sup>, D. Kumar<sup>2</sup> and Ashok S. Chouhan<sup>2</sup>**

<sup>1</sup>*Department of Chemistry, GLA University, Mathura-281406*

<sup>2</sup>*Centre of Research for Chemical Sciences, Govt Model Science College, Jiwaji University, Gwalior - 474009*

*E-mail : rayeesbinahad@gmail.com*

A novel Schiff base, S-Benzyl  $\beta$ -(N-3,5-dichloro-2-hydroxybenzylidene)dithiocarbazate (sbcsa), was synthesized and characterized by FT-IR, Raman, UV-Vis, <sup>1</sup>H NMR, and mass spectrometry. Docking studies revealed notable binding affinities of HL with DNA (−19.66 kJ/mol), protein 3C5W (−20.50 kJ/mol), and SARS-CoV-2 main protease 7BRO (−4.8 kJ/mol), suggesting its potential as a COVID-19 main protease inhibitor. HL exhibited antibacterial activity against multidrug-resistant *E. coli* (Gram-negative) and *S. aureus* (Gram-positive). Thermal analysis under nitrogen atmosphere confirmed stability up to 500/ °C. Density functional theory (DFT) calculations using RB3LYP/6-311++G(d,p) optimized HL geometry, yielding a minimum energy of −2480.6125 a.u. and a dipole moment of 0.6776 D. Experimental and theoretical vibrational spectra were correlated using VEDA-4 and Gaussian09, revealing 96 fundamental modes and potential energy distribution (PED) contributions. Dihedral angle analysis indicated a non-linear molecular geometry. These findings support the utility of HL and its metal complexes in bioinorganic and electronic applications.

## IO-13: Detecting Platinum in Biological Systems

Raj Kishore Shukla<sup>1</sup> and Prathibha Tripathi<sup>2</sup>

<sup>1</sup>Atarra P G College Atarra Banda

<sup>2</sup>Pandit Kedarnath Rajaram Mahavidyalaya Kamasin, Banda

E-mail: st0312@gmail.com

The study of platinum(II) complexes and their interactions with biological molecules has prompted the development of various analytical techniques to detect platinum and analyse its bonding.

Methods of Detection : Direct detection methods include flameless atomic absorption spectroscopy (AAS), which is cost-effective, versatile, and capable of detecting 1-20 micrograms of platinum, even in the presence of biopolymers, provided other metals are absent. Another direct approach uses the radioactive isotope <sup>195m</sup>Pt, enabling precise measurement of platinum-such as cis-[Pt(NH<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>]-bound to DNA. Advanced instrumental techniques provide more detailed structural information. EXAFS (Extended X-ray Absorption Fine Structure) allows measurement of distances between platinum atoms and their ligands on DNA. Mass spectrometry is applied to investigate platinum binding to nucleosides. These methods help determine both the quantity and mode of platinum binding. Colorimetric tests also offer qualitative insights, as some platinum-biopolymer complexes generate distinctive spectral bands absent in the unbound components. Such shifts in absorption or appearance of new peaks can serve as indicators of complex formation. Together, these methods-spanning simple spectroscopic techniques to specialized isotopic and structural analyses-provide essential tools for detecting platinum in biological systems and understanding its biochemical interactions.

## IO-14: Metal Complexes of Schiff Base: Synthesis, Spectral Characterization, and Antibacterial Evaluation

Shalini Yadav\* and Vinod Kumar\*\*

Department of Chemistry, Agra College, Agra - 282004

E-mail : yadavshalini628@gmail.com\*; vinodkchem@gmail.com\*\*

A novel Schiff base nicotinic acid [1-(3,4-dimethoxyphenyl)ethylidene]hydrazide, was synthesized by refluxing 3,4-dimethoxyacetophenone with nicotinic hydrazide in ethanol. Its Co(II), Ni(II), Cu(II), and Fe(III) complexes were subsequently prepared. The ligand and its metal complexes were characterized using infrared (IR) spectroscopy, <sup>1</sup>H NMR, elemental analysis, electronic spectroscopy, magnetic measurements, and X-ray diffraction technique (XRD). The synthesized compounds were also evaluated for their antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*.

## **IO-15: Synthesis and Characterization of Metal Complexes with PET- derived Aromatic Amide Ligands**

**Vishu Sharma and R. K. Soni**

*Department of Chemistry, Ch. Charan Singh University, Meerut*

*E-mail : vishusharma190398@gmail.com*

The synthesis of metal complexes using ligands derived from recycled polymers offers a sustainable route toward high-value inorganic materials. In this study, aromatic amide ligands obtained from polyethylene terephthalate (PET) waste were utilized for the preparation of metal complexes. The coordination behavior of the ligands toward the metal ions was investigated using FTIR, UV-Visible, NMR, and elemental analysis, confirming effective metal-ligand interactions through the amide and aromatic donor sites. The resulting complexes exhibited good stability and distinct structural and optical characteristics compared with the parent ligand, as evidenced by their spectroscopic features. Preliminary assessments indicate functional attributes that suggest potential for advanced material and biological applications. This work demonstrates the feasibility of integrating inorganic complex formation with polymer waste valorization, contributing to the development of sustainable, multifunctional materials.

## **IO-16: Complexes of Fe(III) and Co(III) with Macrocyclic Schiff base derived from 4-chloro-1,2-phenylenediamine and 2,6-diacetylpyridine: Synthesis, Characterization and Molecular Docking Studies**

**Manju Yadav<sup>1,2</sup> and V. K. Sharma<sup>1\*</sup>**

*<sup>1</sup>Department of Chemistry, University of Lucknow, Lucknow - 226007 (UP)*

*<sup>2</sup>Department of Chemistry, M. P. Govt. P. G. College, Hardoi (UP)*

*E-mail : vksharma21@hotmail.com; ochemmanju@gmail.com*

This study highlights the synthesis and characterization of macrocyclic Schiff base complexes of Fe(III) and Co(III) with macrocyclic Schiff base derived from 4-chloro-1,2-phenylenediamine and 2,6-diacetylpyridine. The complexes were synthesized by the template method. The alcoholic solution of hydrated Fe(III)chloride was refluxed with 4-chloro-1,2-phenylenediamine to obtain a metal amine adduct, which was further refluxed with 2,6-diacetylpyridine to get the complex. For the synthesis of Co(III) complex, the alcoholic solution of CoCl<sub>2</sub>.6H<sub>2</sub>O was refluxed with diamine in the presence of 30% H<sub>2</sub>O<sub>2</sub> solution, followed by refluxing with 2,6-diacetylpyridine. The complexes

were characterized by elemental analysis, FTIR and UV-Visible spectroscopy. Moreover, magnetic susceptibility measurements and molar conductances of synthesized complexes were also determined. The synthesized complexes were screened for their antimicrobial activity in vitro against two gram-negative bacteria, *Pseudomonas aeruginosa*, *Escherichia coli* and the fungi *Candida albicans* and *Aspergillus niger*, by the agar well diffusion method. It has been found that the metal complexes  $\text{Co(III)L}^1$  and  $\text{Fe(III)L}^1$  have stronger antifungal activity. The macrocyclic complex  $\text{Co(III)L}^1$  has the highest antifungal activity against *C. albicans* (IZD=21mm).  $\text{Fe(III)L}^1$  also has the same trend for antifungal activity. Both complexes were docked with the receptor proteins of *E. coli* (PDB ID:1kzn), *P. aeruginosa* (PDB ID: 4cl6), and *C. albicans* (PDB ID: 5fsa) and it was observed that  $\text{Co(III)L}^1$  and  $\text{Fe(III)L}^1$  both have the highest binding affinity with receptor protein of *C. albicans* (PDB ID: 5fsa), -11.8 and -13.0 Kcal, respectively.

### **IO-17: Development of a Metallophillic Organopalladium (II) complex bearing SeCSe type trans pincer ligand: A $(\text{Se}^{\text{II}})_2 \cdots \text{Pd}^{\text{II}} \cdots \text{Pd}^{\text{II}} \cdots (\text{Se}^{\text{II}})_2$ Interactions**

**Puspendra Singh<sup>1\*</sup>, Amit K. Tripathi<sup>1</sup>, Roop Kumar<sup>1</sup> and Ray J. Butcher<sup>2</sup>**

<sup>1</sup>*Department of Chemistry, Dr. Shakuntala Misra National Rehabilitation University, Lucknow - 226017*

<sup>2</sup>*Department of Chemistry, Howard University, Washington DC 20059, USA.*

<sup>\*</sup>*E-mail : pushpendrasingh0612@gmail.com*

Bromination of 5-tert-Butyl-1,3-xylene with N-bromosuccinamide in the presence of AIBN produced the 5-tert-Butyl-1,3-bis(bromomethyl) benzene (1) as colorless crystals. The reaction of in situ generated  $\text{PhSe}^+$  with 1 has resulted in the formation of SeCSe type trans pincer ligand, ((5-(tert-butyl)-1,3-phenylene) bis(methylene)) bis(phenylselane) (2). The trans pincer ligand 2 reacted with  $\text{Na}_2\text{PdCl}_4$ , can afford a metallophillic organopalladium(II) complex (3) with good yield. Compounds 1, 2 and 3 have been characterized by  $^1\text{H}$  NMR,  $^{13}\text{C}\{^1\text{H}\}$  NMR, and elemental analysis. Further, compound 3 was also characterized by single crystal X-ray studies. Molecular structure of 3 exhibits two Pd-Se bonds (2.395(1) and 2.410(0) Å) due to the trans influence of two Se donor atoms on each other and the rigidity of ligand 2. In the crystal packing diagram of 3, a dimeric unit is formed due to  $(\text{Se}^{\text{II}})_2 \cdots \text{Pd}^{\text{II}} \cdots \text{Pd}^{\text{II}} \cdots (\text{Se}^{\text{II}})_2$  type metallophillic interactions. In addition to these interactions C-H'  $\cdots$  Cl hydrogen bonding interactions also play a significant role in the self-assembly of 3.

## IO-18: Synthesis, Characterization, Biological Activity and Molecular Docking of Schiff base Derived from o-vanillin and its Complexes

Ashok Singh and Nand Lal\*

Department of Chemistry, V.S.S.D. College, Kanpur, U.P.

E-mail : drnandlal71@gmail.com

This study highlights the synthesis and characterization of a tetradentate ONNO donor Schiff base ligand H<sub>2</sub>L (Bis-[3-methoxysalicylidine]-4-nitro-1,2-phenylenediamine) and its complexes with Co(II), Cu(II) and Ni(II). The Schiff base ligand was synthesized by condensation of a 1:1 alcoholic solution of o-Vanillin (3-methoxysalicylaldehyde) and 4-Nitro-1,2-phenylenediamine. The ligand and complexes were characterized by elemental analysis, FTIR, UV-Visible <sup>1</sup>H NMR and <sup>13</sup>C NMR spectroscopy. Moreover, magnetic susceptibility measurements and molar conductances of synthesized ligand and complexes were determined. Furthermore, synthesized ligand and complexes were screened for their antimicrobial activity in vitro against two gram-negative bacteria, *Pseudomonas aeruginosa*, *Escherichia coli* and one gram-positive bacterium, *Staphylococcus aureus*, by agar well diffusion method. It was observed that the biological activity of the complexes was greater than that of the ligand. The in silico anticancer activity of ligand and complexes was carried out with Human breast cancer protein HER2(PDB ID: 3MZW) by molecular docking and the results support that the CoL complex has the best inhibition property towards HER2 (Binding energy = -9.2).

## IO-19: Ultrastable Biimidazoline-Based MOFs for Smartphone-Assisted Ratiometric Fluorescent Sensing of Nitrofurazone and Trinitrophenol

Yu Wu<sup>1</sup>, Muhammad Shofiyullah<sup>2</sup> and Abhinav Kumar<sup>2\*</sup>

<sup>1</sup>School of Chemistry and Environmental Engineering, Sichuan University of Science & Engineering, Zigong, 643000, PR China

<sup>2</sup>Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow - 226007

E-mail : abhinavmarshal@gmail.com

Three Cd(II)-based coordination frameworks, [Cd(H<sub>2</sub>L)(H<sub>2</sub>O)·3H<sub>2</sub>O] (1), [Cd(L)<sub>0.5</sub>(2,2'-bipy)] (2), and [Cd(L)<sub>0.5</sub>(phen)·1.25H<sub>2</sub>O] (3), were synthesized using 1,1'-di(3,5-dicarboxylbenzyl)-2,2'-biimidazoline (H<sub>4</sub>L) with auxiliary diimine ligands. Single-crystal X-ray diffraction reveals that 1 exhibits a 3D sra topology with large accessible voids, while 2 and 3 crystallize in CdSO<sub>4</sub>-type networks, their architectures modulated by the  $\pi$ -conjugated co-ligands. The frameworks exhibit intense ligand-centered luminescence that is effectively quenched by nitrofurazone



(NFZ) and 2,4,6-trinitrophenol (TNP), showing Stern–Volmer constants in the  $10^{10}\text{M}^{-1}$  range and submicromolar detection limits (0.17–0.30  $\mu\text{M}$ ). Detailed mechanistic studies including UV–Vis spectral overlap, molecular orbital analysis, Hirshfeld mapping, and void volume correlation confirm that the fluorescence quenching occurs through a synergistic mechanism involving photoinduced electron transfer, Förster resonance energy transfer, and the inner filter effect, further enhanced by hydrogen bonding and framework porosity. Real water sample analysis shows excellent detection accuracy with recoveries of 95–110% and RSD values below 5%. 1 displays the most balanced sensitivity and robustness, 3 shows high NFZ selectivity, and 2 is efficient for TNP sensing. A smartphone-based detection platform further demonstrates the feasibility of portable and intelligent NFZ/TNP monitoring.

## **IO-20: DNA Binding, Anticancer, Antifungal, and Antibacterial Activities of Ru(II) Complexes Supported by In-Silico Studies**

**Saniya Firdaus<sup>1</sup>, Swaila Bano<sup>1</sup>, Divya Singh<sup>2</sup>, Harshita Gaurav<sup>2</sup>, Amritesh Chandra Shukla<sup>2</sup>, Anushka Bari<sup>3</sup>, Sudheer Kumar Singh<sup>3</sup> and Ashok K. Singh<sup>1\*</sup>**

<sup>1</sup>*Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow-226007*

<sup>2</sup>*Department of Botany, Faculty of Science, University of Lucknow, Lucknow-226007*

<sup>3</sup>*Division of Molecular Microbiology and Immunology, CSIR-Central Drug Research Institute, Lucknow - 226031*  
E-mail: singhpus01@gmail.com

The Ru complexes (LM1), (LM2), and (LM3) were synthesized by using N-substituted benzophenone thiosemicarbazone ligands (L1, L2, L3). The condensation of 2-hydroxy-4-methoxy benzophenone and N-substituted thiosemicarbazide resulted in these ligands. These ligands and complexes were characterized by elemental analysis, FT-IR, <sup>1</sup>H, <sup>13</sup>C-NMR, UV-Vis, and HR-MS spectroscopy. The spectral data confirm the ligand coordinating through tridentate fashion via the imine nitrogen, thioamide sulfur, and phenolic oxygen atom of the benzophenone moiety. The geometry was optimized by theoretical calculation using DFT, and the structure reveals that RM1-RM3 adopt an octahedral geometry. Molecular electrostatic potential (MEP), HOMO-LUMO analysis provided insights into the electronic characteristics and stability of the complexes. Moreover, DNA binding studies were conducted with all complexes and binding constants (K<sub>b</sub>) were found, i.e., of  $6.43 \times 10^3 \text{ M}^{-1}$  (LM1),  $3.51 \times 10^3 \text{ M}^{-1}$  (LM2), and  $4.92 \times 10^3 \text{ M}^{-1}$  (LM3). It was found that DNA binds in a minor groove mode,

which is also supported by in-silico docking studies. In vitro antibacterial efficacy of the compounds was tested against *Mycobacterium tuberculosis* H37Ra bacterial strains. Additionally, the antifungal activity of the conjugate complexes was evaluated against *Fusarium solani*. To enhance the bioefficacy of the complexes, anticancer activity was evaluated against A549 (human lung carcinoma) cancer cell lines using the MTT assay. ADME analysis indicates that the synthesized complexes exhibit drug-like characteristics, with acceptable metabolic stability and safety profiles.

## **IO-21: Ag-Embedded Composites Ag-ZnO Nanostructures for Sustainable Solutions: Synergistic Photocatalytic Degradation and Antioxidant Efficacy**

**Gulab Gugale<sup>1\*</sup>, Vivekanand Jawale<sup>2</sup> and Sunil Hande<sup>3</sup>**

*<sup>1</sup>Department of Chemistry, Haribhai V. Desai College of Commerce, Arts and Science, Pune - 411002*

*<sup>2</sup>Modern College of Engineering, Shivajinagar, Pune*

*E-mail : gsgugale02@gmail.com<sup>1</sup>; vivekjawale25@gmail.com<sup>2</sup>*

This study explores the dual-functional potential of silver-embedded zinc oxide (ZnO) nanocomposites with varying silver content (1, 3, and 5 wt.%) for enhanced photocatalytic and antioxidant applications. Initially, pure ZnO nanostructures were synthesized under controlled reaction parameters, revealing hexagonal rod-like morphologies via FESEM and TEM analyses. XRD confirmed their crystalline wurtzite structure, while UV-Vis spectroscopy indicated a bandgap of 3.27 eV (absorption at 380 nm). Increasing reaction parameters induced morphological evolution into three-dimensional distorted spherical structures. Photocatalytic evaluation under UV light demonstrated superior degradation of Rhodamine 6G (R6G) by the 5 wt.% Ag-ZnO composites, achieving 93.36% efficiency with a rate constant of  $6.54 \times 10^{-3} \text{ min}^{-1}$ . This composite also exhibited remarkable recyclability, retaining >91% activity after five cycles. Antioxidant assessments (DPPH, ABTS, FRAP, FIC) highlighted the 5 wt.% Ag-ZnO's exceptional radical scavenging capacity, underscoring its dual functionality.

## **IO-22: Elevating the Wastewater Treatment Performance of Loose Nano-filtration Membranes using Natural Clay Functionalized with $\text{AlFe}_2\text{O}_4$ Nanocleaners**

**Ashok Shrishail Maraddi and S. K. Nataraj\***

*Centre for Nano & Material science, Jain Global Campus, Jain University,  
Jakkasandra Post, Ramanagara, Bangalore - 562112*

*E-mail : s.ashok@jainuniversity.ac.in; sk.nataraj@jainuniversity.ac.in*

Membranes with right recipe can potentially give exceptionally high product water flux with high rejection, recovery ratio, prolonged life with anti-fouling capabilities, low operating costs, and low operating expenses. In this regard, an innovative  $\text{AlFe}_2\text{O}_4$  functionalized bentonite ( $\text{AlFe}_2\text{O}_4\text{@BT}$ ) was prepared to be used as performance boosting agent in Polyethersulfone (PES)-based mixed matrix loose nanofiltration membrane (LNM). Herein, the fabrication PES-based mixed achieved by blending different wt.% of  $\text{AlFe}_2\text{O}_4\text{@BT}$  material through phase inversion technology. The effects of  $\text{AlFe}_2\text{O}_4\text{@BT}$  on the structure and functionality of the new material  $\text{AlFe}_2\text{O}_4\text{@BT}$ -PES NLMS were thoroughly examined by scanning electron microscopy, contact angle, antifouling measurements and so on. The Separation efficiency of  $\text{AlFe}_2\text{O}_4\text{@BT}$ -PES based LNM was recorded up to 80%, 85% and 95% of Crystal violet (CV), Congo Red (CR), and humic acid, respectively with exceptional high product flux efficiencies and anti-fouling properties to commercial polyamide membranes. The new LMMs operate at relatively low operating pressure (1-4 bar) which makes them sustainable separation process with lower flux decline ratio and high recovery ratio making it superior membrane material combination.

## **IO-23: Bio-Waste-Derived Graphene Nanomaterials for Inhibition of Airborne Microorganisms**

**Mohammad Ikbal and Ranjit Kumar**

*Department of Chemistry, Faculty of Science, Dayalbagh Educational Institute  
Dayalbagh, Agra-282005*

The rising abundance of bioaerosols airborne particles containing microorganisms or their fragments poses substantial challenges to public health, environmental integrity, and climate stability. Conventional mitigation strategies often struggle with limitations in cost-effectiveness, scalability, and ecological sustainability. To overcome these barriers, this study adopts a sustainable route for the synthesis of graphene-based nanomaterials from bio-waste precursors and evaluates their potential to suppress the biological components of ambient aerosols. Agricultural residues such as

coconut shells, sugarcane bagasse, and rice husk were utilized as inexpensive, renewable feedstocks for the production of high-quality graphene with tunable physicochemical characteristics. Bio-waste-derived graphene (BWG) was synthesized through pyrolysis of agricultural residues followed by chemical activation to enhance surface area and reactivity. The produced graphene sheets were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), to assess structural, morphological, and crystalline features. Antimicrobial and antifungal activities were tested against airborne bacterial and fungal strains commonly found in urban and semi-urban aerosols. Laboratory chamber experiments simulated ambient aerosol conditions, enabling direct BWG microbe interactions. Field trials were conducted at an urban site to evaluate real-world bioaerosol reduction efficiency. Laboratory results demonstrated strong microbial inhibition via membrane disruption, oxidative stress induction, and physical adsorption. Antimicrobial efficiency was positively correlated with the presence of surface functional groups and edge defects in BWG. Field trials confirmed a measurable reduction in culturable bioaerosol concentrations upon BWG exposure. This work provides dual environmental benefits by valorizing agricultural bio-waste into advanced nanomaterials and mitigating airborne biological pollutants.

## **IO-24: Pd-catalyzed Synthesis of Benzoxazolone Derivatives and In-silico Study Targeted TSPO Protein for Neuro-inflammation Treatment**

**Nidhi, Khushboo Singh and Vinay Kumar Singh\***

*Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow - 226007, U.P.*

*E-mail : vinayksingh.lu@gmail.com; nidhichemistry27@gmail.com; khushboobkt3@gmail.com*

Benzoxazolones are multifaceted heterocyclic structures recognized for their diverse range of biological effects, such as anti-inflammatory, antimicrobial, and anticancer properties. In this study, we established an effective palladium-catalyzed carbonylative cyclization approach for the creation of substituted 2(3H)-benzoxazolones utilizing o-haloanilines and o-aminophenols. The reaction occurs under mild conditions with the use of Pd(OAc)<sub>2</sub> and phosphine ligands alongside CO, resulting in the desired heterocycles being produced in good to excellent yields. This method demonstrates a wide range of substrate applicability, tolerance of various functional groups, and ease of operation, thus making it ideal for the quick synthesis of bioactive analogs. Translocator Protein

(TSPO, 18kDa) is found throughout the outer mitochondrial membrane and is notably abundant during the activation of microglia in neuroinflammatory disorders. The translocator protein (TSPO, 18kDa) serves as a highly valuable biomarker for investigating the impact of neuroinflammation in both humans and different animal species. In-silico analyses of synthesized benzoxazolone derivatives indicated strong interactions with translocator proteins. These results imply that benzoxazolone derivatives could serve as a potential marker for the visualization of neuroinflammation through targeting TSPO.

## **IO-25: Fe(III)-Catalyzed Synthesis of Benzimidazole Compounds and In-Silico Study for Non-melanoma Skin Cancer Treatment**

**Vinay Kumar Singh\* and Arpit Srivastav**

*Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow-226007, U.P.*

*E-mail : vinayksingh.lu@gmail.com; arpitsri7054@gmail.com*

Benzimidazole derivatives are a crucial class of nitrogen-containing heterocycles with a diverse range of pharmaceutical and material applications. In this study, a metal-catalyzed method was utilized to synthesize benzimidazole using o-phenylenediamine and aromatic aldehydes effectively. A transition metal complex, such as Fe(III), catalyzed the process in mildly oxidative conditions. Compared to traditional acid- or oxidant-mediated syntheses, the metal-catalyzed technique showed excellent atom economy, operational simplicity, and less environmental impact, making it an appealing pathway for the sustainable synthesis of benzimidazole scaffolds.

Non-melanoma skin cancer (NMSC) is the fifth most common cancer. NMSC originates from keratinocytes. Ultraviolet light plays an important role as an initiator and promoter of NMSC. Treatment of NMSC includes drug 5-fluorouracil, imiquimod, diclofenac, ingenol, mebutate, resiquimod, betulinic acid, vismodegib, and cytotoxic chemotherapy. Epidermal Growth Factor Receptor (EGFR) tyrosine kinase inhibitor plays an essential role in the development of treatment of cancer. Compounds showing anticancer activities against NMSC are evaluated through in-silico studies of the compound via targeting various EGFR proteins and in vitro analysis.

## **IO-26: Insights into the Supramolecular and Molecular Electrocatalytic Properties of 1,2-bis(diphenylphosphine)Ethane Appended Nickel(II) 1,2-dithiosquarate for Oxygen and Hydrogen Evolution Reactions**

**Aparna Kushwaha<sup>1</sup>, Devyani Srivastava<sup>1</sup>, Gabriele Kociok-Kohn<sup>2</sup> and Abhinav Kumar<sup>1</sup>**

<sup>1</sup>*Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow-226 007*

<sup>2</sup>*Department of Chemistry, BBDNIIT, Lucknow-226 028*

<sup>3</sup>*Physical Structure Characterization, University of Bath, Claverton Down, Bath BA2 7AY, UK*

*E-mail : devyanisri05@gmail.com*

A new heteroleptic Ni(II) dithiolate [Nidppe(dtsq)] (Nidtsq) (dppe = 1,2-bis-(diphenylphosphino)ethane, dtsq2 = 3,4-dioxocyclobut-1-ene-1,2-dithiolate) has been synthesised and characterized spectroscopically and by single crystal X-ray diffraction. The single crystal X-ray diffraction study reveals asquare planar geometry around the Ni(II) center wherein dtsq2 and dppe ligands exhibit bidentatechelating coordination modes by their respective sulfur and phosphorus centers. The solid-stateframework of Nidtsq is stabilized by C–H $\cdots$ O, C $\cdots$ H, C $\cdots$ O and  $\pi\cdots\pi$  intermolecular interactions and the complex displays an interesting pair of intramolecular C–H $\cdots$ Ni anagostic interactions. Furthermore, the electrocatalytic properties of Nidtsq have been assessed for the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). The electrocatalytic properties of Nidtsq have been found to be better than those of the previously reported Nidtsq complex. In the OER, the complex displayed an overpotential of 0.37 V with  $\eta^{10}$  of 414 mV and a Tafel slope of 237 mVdec<sup>-1</sup> and in the HER it exhibited an overpotential of 0.35 V with  $\eta^{10}$  of 670 mV and a Tafel slope of 368 mV.dec<sup>-1</sup>.

## **IO-CYSA-01: Chelation of Life-Essential Metal-ions Co(II) and Zn(II) with a synthesized Bioactive Ligand: Synthesis, Structural Characterization, and Antimicrobial Evaluation**

**Ankit Kumar Choubey<sup>\*</sup> and A. P. Mishra**

*Department of Chemistry, Dr. Hari Singh Gour Vishwavidyalaya (A Central University), Sagar - 470003, M.P.*

*E-mail : ankit.choubey94@gmail.com; apmishrasagar@gmail.com*

Bioactive ligands incorporating the imine (C=N) functional moiety constitute a structurally versatile and pharmacologically significant

class of compounds, primarily due to their pronounced chelating ability toward diverse metal ions. Building upon our earlier investigations on transition metal complexes of a bioactive Schiff base ligand, the present study delineates the synthesis and coordination characteristics of 2-((5-bromo-2-methoxybenzylidene)amino)-6-chloro-4-nitrophenol (L) with biologically relevant Co(II) and Zn(II) ions. The resulting mononuclear metal complexes were systematically synthesized and comprehensively characterized through FT-IR, UV-Vis, NMR, thermogravimetric analysis (TGA), and cyclic voltammetry (CV) techniques. Coordination was evidenced by a characteristic downfield shift in the azomethine (C=N) stretching band from 1668  $\text{cm}^{-1}$ , confirming metal–nitrogen bond formation. Electrochemical characterization via CV indicated a quasi-reversible one-electron redox process, signifying the electroactive nature of the complexes. Spectroscopic and analytical data collectively suggest a distorted octahedral geometry around the central metal ions. The complexes displayed appreciable solubility in polar aprotic solvents such as DMSO and DMF. In-vitro biological evaluation demonstrated notable antimicrobial potential, wherein the Co(II) complex exhibited superior antifungal and antioxidant activities relative to its Zn(II) analogue. These findings underscore the pronounced biofunctional versatility of this ligand framework, extending its coordination and biological applicability beyond its previously reported Ni(II) and Cu(II) congeners.

## **IO-CYSA-02: Enhanced Photocatalytic Hydrogen Evolution using Heterostructured Material (CoVLDH/CeS<sub>2</sub>) with Efficient Charge Separation**

**Aditya Hadrihalli, M. Sreenivasulu and Nagaraj P. Shetti\***

*Center for Energy and Environment, School of Advanced Sciences,  
KLE Technological University, Hubballi-580031, Karnataka  
E-mail : npshetti@kletech.ac.in*

In search of developing cutting-edge photocatalysts for sustainable and clean hydrogen generation via water splitting, we investigated developing a highly effective and stable S-scheme heterojunction photocatalyst as a highly efficient catalyst for water splitting. In this research, visible-light-driven hydrogen (H<sub>2</sub>) evolution with the help of cobalt-vanadium layered double hydroxide (CoVLDH), combined with cerium disulfide (CeS<sub>2</sub>)-based heterostructured CoVLDH/CeS<sub>2</sub> nanocomposites, was prepared. The material was fully characterized by XRD, FESEM, and TEM measurement, which offered an exceptional H<sub>2</sub> evolution rate of 16.89  $\text{mmol.h}^{-1}.\text{g}^{-1}$ , outperforming nearly two times that of the neat CoVLDH optimized CoVLDH/CeS<sub>2</sub> nanocomposite. Reaction time,



sacrificial reagents, and photocatalyst dosage were systematically optimized to prove the effectiveness of the potential of the material. The strong interfacial coupling between CoVLDH and CeS<sub>2</sub> enabled the effective charge separation, directed electron transmission, and suppression of electron–hole recombination via the S-scheme mechanism due to its increased photocatalytic action. Additionally, the nanocomposite had an outstanding photostability over an extended exposure to radiation. The research highlights the potential of transition-metal LDH/sulfide-based heterostructures as viable options for highly efficient solar-to-hydrogen energy conversion.

### **IO-CYSA-03: Nickel Bismuth Selenide (Ni<sub>3</sub>Bi<sub>2</sub>Se<sub>2</sub>) Anchored Mxene Hybrid Composite Electrode for Symmetric Supercapacitor**

**Milind D. Babar, Amol B. Tambe, Aman R. Pathan and Satish K. Pardeshi\***

*Department of Chemistry, Savitribai Phule Pune University (formerly University of Pune), Ganeshkhind, Pune - 411007*

*E-mail : satish.pardeshi@unipune.ac.in*

Chalcogenide hybrids (CHs) have emerged as promising candidates for next-generation energy storage devices (ESDs), owing to their excellent redox activity, structural stability, cost-effectiveness, and superior electrical conductivity. In this study, a novel hybrid chalcogenide material composed of Mxene and Nif Bi, Se, (NBSe) was successfully synthesized via a straightforward hydrothermal method. This synthesis approach significantly enhances the electrochemical performance of the resulting NBSe/Mxene composite. Structural analysis using X-ray diffraction (XRD) confirms the effective anchoring of NBSe nanogranules onto the Mxene surface, as evidenced by changes in lattice constants, crystallite size, and microstrain. The hybrid's enlarged surface area facilitates rapid ion transport and contributes to its high specific capacitance and exceptional cycling stability. Notably, the NBSe/Mxene electrode retains approximately 94% of its initial capacity after 10,000 charge-discharge cycles, demonstrating its long-term durability. Furthermore, a symmetric supercapacitor device using NBSe/Mxene//NBSe/Mxene electrodes was fabricated and tested to evaluate practical applicability. The device exhibited outstanding specific energy and power characteristics, underscoring the potential of NBSe/Mxene hybrids as high-performance electrode materials for advanced ESDs.

## **IO-CYSA-04: Synthesis, Characterization and Biological Activity of Pyruvic Acid Hydrazone Derivative and its Transition Metal Complexes**

**Divya Hegde<sup>1,2</sup> and K. B. Gudasi<sup>1</sup>**

<sup>1</sup>*Department of Chemistry, Karnatak University, Dharwad-580 003*

<sup>2</sup>*Department of Chemistry, MES's M. M. Arts and Science College, Sirsi -581402 (U.K.)*

*E-mail : divya4star@gmail.com*

There has been burgeoning interest in the investigation of hydrazones of pyruvic acid derivatives and has received attention because of their pharmacological like antiproliferative, physiological properties and their ability to afford stable bonds with transition metal ions. Encouraged by these reports and in continuation of our search for biologically active pyruvic acid derivatives, we report this article. In this work, we are presenting a novel hydrazone derived from pyruvic acid, 'ethyl 2-(2-(2-methylbenzoyl)hydrazono)propanoate' and its transition metal complexes were synthesized and characterized by various spectroscopic (<sup>1</sup>H, <sup>13</sup>C, 2D HMQC NMR, FT-IR, mass and UV-Vis) techniques, elemental, conductivity measurements and thermo gravimetric analysis. The single crystal X - Ray diffraction study of the ligand was shown to be orthorhombic crystal system with Pna2(1) space group, having 4 ligand molecules in a unit cell. The interaction of synthesized compounds with CT-DNA and pBR322 DNA were studied. The in vitro antiproliferative studies suggest that ligand and copper complex exhibit significant cytotoxic activity on KB, and A-431 cell lines compared to MCF-7, Mia-Pa-Ca-2 K-562, A-549 and VERO cell lines.

## **IO-CYSA-05: Synthesis, Structural Investigations, DFT Interpretations, Cytotoxic Evaluation and Colorimetric Chemo Sensor Applications of novel azo Dyes**

**Khushi Siri C.N. and Shoukat Ali R.A.\***

*Department of Studies and Research in Chemistry, Davangere University, Shivagangotri, Davangere-577007 Karnataka*

*\*E-mail : kscn2024@gmail.com; drsardvg2022@gmail.com.*

The present research describes a series of novel azo dyes derived from 5-aminoindan [4a-4e], which are synthesized through diazotization and coupling reactions. Various phenolic and heterocyclic substrates, are used as coupling components for the preparation of title compounds. The structural investigations of the synthesized compounds were carried out by comprehensive spectral characterization techniques like UV-Visible, FT-IR and <sup>1</sup>H NMR, including LC-MS analyses. Density

Functional Theoretical (DFT) studies provide the energy gap [ $\Delta E = E_{\text{HOMO}} - E_{\text{LUMO}}$ ] and other various electronic properties. Colorimetric - Chemo sensing ability of synthesized azo dyes for the detection of transition metal ions [ $\text{Fe}^{+2}$ ,  $\text{Ni}^{+2}$ ,  $\text{Cu}^{+2}$  and  $\text{Zn}^{+2}$ ] and heavy metal ions like  $\text{Pb}^{+2}$  and  $\text{Hg}^{+2}$  were investigated. Further the synthesized compounds were screened for their cytotoxic potential against the A431 human skin carcinoma cell lines via MTT assay. Where the compounds 4c and 4d exhibited dose dependant cytotoxic activity. The present research work introduces new azo dyes which has both biomedical and chemo sensing applications.

## **IO-CYSA-06: In-Situ Growth of Hexagonal $\text{SnS}_2$ Nanoplates on 2D $\text{Ti}_3\text{C}_2\text{T}_x$ : Highly efficient Nano-heterostructure for Hydrogen Generation and Dye Degradation**

**Amol B. Tambe and S. K. Pardeshi\***

*Department of Chemistry, Savitribai Phule Pune University (formerly University of Pune), Ganeshkhind, Pune-411007*

*\*E-mail : satish.pardeshi@unipune.ac.in*

The successful in-situ synthesis of 2D  $\text{Ti}_3\text{C}_2\text{T}_x/\text{SnS}_2$  nano-heterostructures with different Ti/Sn ratios were demonstrated in this study. These nano-heterostructures were subsequently assessed as photocatalysts for the production of hydrogen by water splitting and dye degradation. The creation and characteristics of the nano-heterostructures were verified using a variety of characterisation techniques. The XRD investigation verified the effective synthesis of  $\text{Ti}_3\text{C}_2\text{T}_x/\text{SnS}_2$  nano-heterostructures by revealing diffraction peaks corresponding to MXene and  $\text{SnS}_2$ . FE-SEM, FETEM, and XPS further confirmed the development of 2D nano-heterostructures, revealing layered structures of MXene and hexagonal nanosheets of  $\text{SnS}_2$ .  $\text{Ti}_3\text{C}_2\text{T}_x$  and  $\text{SnS}_2$  were found to coexist in the nano-heterostructures, according to high-resolution TEM images and specific area electron diffraction patterns. Optical characteristics of the nano-heterostructures revealed band gaps between 2.17 to 2.34 eV, absorption in the visible light spectrum. All compositions demonstrated band edge emission in the 535-550 nm range in photoluminescence (PL) spectra, with the exception of the pure  $\text{Ti}_3\text{C}_2\text{T}_x$ . At around 1178.5  $\mu\text{mol}/0.1\text{ g}$ , the TS-5 wt% nano-heterostructure demonstrated the highest photocatalytic hydrogen generation, greatly surpassing other compositions. Effective methylene blue (MB) dye degradation up to 90% and a high apparent quantum yield of 2.2% were also demonstrated. The study emphasizes how the TS-5 wt% nano-heterostructure greater photocatalytic activity is a result of the longer decay durations of its photogenerated charge

carriers. Based on these findings, photocatalytic effectiveness can be greatly increased by designing 2D nano-heterostructures with an optimal composition.

### **IO-CYSA-07: Electrochemical Trace Detection of 2,4-Dichlorophenoxyacetic Acid Using an Fe-Doped WO<sub>3</sub> Matrix-Modified Electrode**

**Hiregowdara Sushma and Nagaraj P. Shetti\***

*Centre for Energy and Environment, School of Advanced Sciences, KLE Technological University, Hubballi-580031, Karnataka  
E-mail : npshetti@kletech.ac.in; sushmah.jee@gmail.com*

The excessive application of pesticides in agricultural practices has led to significant environmental contamination and adverse health effects. In this work, Fe-doped tungsten oxide (WO<sub>3</sub>) nanostructures were synthesised and utilised as inorganic modifiers for developing a carbon-based electrochemical sensor for the detection of the synthetic growth regulator 2,4-dichlorophenoxyacetic acid (2,4-D). The Fe-doped WO<sub>3</sub> nanoparticles were thoroughly characterised to evaluate their morphology, crystalline features, dopant concentration, elemental distribution, and oxidation states, providing insight into the structural modifications induced by Fe incorporation. The enhanced electrocatalytic activity, high conductivity, and enlarged surface area of the Fe-WO<sub>3</sub>-modified electrode significantly improved the voltametric response compared to the bare carbon paste electrode. Cyclic voltammetry (CV) was employed to study the redox behaviour of 2,4-D, and pH optimisation indicated maximum response at pH 6.0. Electrokinetic and activation parameters were further assessed through sweep-rate- and temperature-dependent analyses to understand the mechanistic aspects of electron transfer on the modified electrode surface. Square wave voltammetry (SWV) enabled highly sensitive detection, achieving a low limit of detection of  $6.28 \times 10^{-8}$  M for 2,4-D. The Fe-doped WO<sub>3</sub>-based sensing platform demonstrates excellent analytical performance and provides a promising inorganic material system for future monitoring of environmentally relevant synthetic growth regulators.

### **IP-01: Synthesis of Rare Metal Oxide Nanoparticles**

**Joshana R. Chaudhari, Bhavana D. Rathod, H. D. Chaudhari and J. J. Vora**

*Department of Chemistry, Hemchandracharya North Gujarat University, Patan-384265, Gujarat  
E-mail : chaudharijes09@gmail.com; haresh09032007@gmail.com*

The synthesis of rare metal oxide nanoparticles (RMO-NPs) a class of materials critical for advanced technologies due to their unique

optical, magnetic and catalytic properties. Traditional synthesis method often suffers from high cost, low yield and poor control over particle size and morphology. This work focuses on developing efficient, scalable, and environmentally benign synthetic routes to produce RMO-NPs with tailored characteristics, explore a combination of solvothermal, co-precipitation, and template-assisted methods, emphasizing precise control over reaction parameters such as Temperature, PH. The aim is to achieve specific morphologies (e.g. nanospheres, nanorods). Characterization techniques including XRD, TEM, EDS confirm the phase purity, crystallinity, size distribution and elemental composition of the synthesized RMO-NPs. The synthesis successfully yielded rare metal oxide NPs with tuneable properties significant potential for applications in catalysis and advanced electronic devices.

### **IP-02: Synthesis, Characterization and Biological Activities of (4-bromo-2-methoxy-6-(((4-phenylthiazole-2-yl)imino)methyl)phenol and its Mn(II), Co(II), Ni(II), Cu(II), Zn(II) and Cd(II) Complex**

**Dhanashri Udhavrao and K. Siddappa\***

*Department of PG Studies and Research in Chemistry, Gulbarga University  
Kalaburagi, Karnataka*

*E-mail : siddappak1965@gmail.com*

The Schiff base ligand (4-bromo-2-methoxy-6-(((4-phenylthiazole-2-yl)imino)methyl)phenol (BMPTIMP) was prepared by via condensation of 2-amino-4-phenylthiazole and 5-bromo-2-hydroxy-3-methoxybenzaldehyde and its Mn(II), Co(II), Ni(II), Cu(II), Zn(II) and Cd(II) Complexes have been synthesized and characterized by elemental analysis, IR, Far IR, UV-Vis, mass spectrometry, <sup>1</sup>H NMR, XRD, and Thermal studies. By these spectral data it is found that Mn(II), Co(II), Ni(II), and Cu(II) complexes shows octahedral geometry whereas Zn(II) and Cd(II) complexes show tetrahedral geometry. The Schiff base (BMPTIMP) and its metal complexes were screened for their Antimicrobial activities.

### **IP-03: Synthesis and Application of Activated Rh(III) Organometallic Complex in the formation of Late-Stage Spirosuccinimide Drug Candidates**

**Rupal Rai<sup>1</sup>, Neeraj Kumar Mishra<sup>1\*</sup> and In Su Kim<sup>2\*</sup>**

*<sup>1</sup>Department of Chemistry, Faculty of Science, University of Lucknow,  
Lucknow-226007, U.P.*

*<sup>2</sup>School of Pharmacy, Sungkyunkwan University, Suwon 16419,  
Republic of Korea.*

*E-mail: neerajchemistry@gmail.com<sup>1\*</sup>; insukim@skku.edu<sup>2\*</sup>*

An activated Rh(III) organometallic complex was synthesized and

evaluated as an efficient catalyst for the late-stage synthesis of spirosuccinimide-based drug candidates. The Rh(III) catalyst, generated through ligand-assisted oxidative activation, effectively promoted selective C–H activation and annulation between N-aryl imides and unsaturated coupling partners. In this transformation, the activated Rh(III) complex facilitates selective C–H activation at the indazolol moiety, followed by insertion of maleimide and intramolecular cyclization to generate the spirocyclic succinimide framework. The reaction proceeds smoothly under mild oxidative conditions with high regioselectivity and functional group tolerance. The resulting spirosuccinimide derivatives are notable for their rigid 3D structures, which enhance biological activity, metabolic stability, and receptor-binding affinity. These properties make them valuable scaffolds for pharmaceutical and medicinal chemistry applications, including the design of anticancer, anti-inflammatory, and CNS-active agents. Thus, this in situ generated activated organometallic Rh(III)-catalyzed methodology represents a sustainable and atom-economical approach for late-stage diversification and synthesis of complex spirocyclic drug-like molecules.

The developed catalytic system exhibits a broad substrate scope and demonstrates its effectiveness in the synthesis of succinimide-containing late-stage spirosuccinimide was performed, which I will present during my poster presentation. This approach highlights practical convenience, sustainability, and significant potential for late-stage drug modification through C–H functionalization.

#### **IP-04: Microstructure Design based on Nano-Hybrids as a High-Performing Electro-Catalyst**

**Bindu B.S.<sup>1</sup>, Ronald Mascarenhas<sup>1</sup>, Shikandar D. Bukkitgar<sup>2</sup> and Nagaraj P. Shetti<sup>2\*</sup>**

<sup>1</sup>Department of Chemistry, St. Joseph's University, Lalbagh Road, Bengaluru – 560027, Karnataka

<sup>2</sup>Centre for Energy and Environment, School of Advanced Sciences, KLE Technological University, Vidyanagar, Hubballi - 580 031, Karnataka  
E-mail: npshetti@kletech.ac.in; bindu2503@gmail.com

The work focused on developing a reduced graphene oxide layer on a carbon matrix through electrochemical methods. The process involved applying a negative potential, initially removing the epoxide and hydroxyl groups, which significantly increased conductivity. The reduced graphene oxide layer developed on the carbon matrix was further decorated with nanostructures, forming a nanohybrid sensor for pharmaceutical detection. The repeatability and reproducibility of the fabricated electrodes were excellent, with RSD% values of 1.8% and 2.4%, respectively. The synergetic effect of nanohybrids facilitated



higher selectivity and sensitivity. Moreover, less interference and high recoveries from the biological matrix made it more suitable for environmental and clinical application trials. The proposed technique was an effective, accurate, time-saving and cost-effective method with good stability.

### **IP-05: Detection of Herbicide Acolbifene Using Graphitic Carbon Nitride (g-C<sub>3</sub>N<sub>4</sub>) Modified Carbon Sensor**

**Rakshita, Davalasab Ilager and Nagaraj P. Shetti\***

*Department of Chemistry, KSS Art's, Science & Commerce College and PG Centre, Gadag-582101, Karnataka  
E-mail: davalasabilager@gmail.com*

Environmental monitoring of water and soil pollutants is associated with a variety of human activities. Escalating demands are therefore emerging for environmental analysis of emerging pollutants, which require the need for more sensitive and selective analytical techniques to alleviate pollution issues. Electro analytical techniques viz., cyclic voltammetry (CV) and square wave voltammetry (SWV) techniques are the widely preferred approaches for quantitative assessment of pollutant such as herbicide acetonifene (ACF). The sensing device was constructed for the detection of ACF using graphitic carbon nitride coated onto glassy carbon electrode (g-C<sub>3</sub>N<sub>4</sub>/GCE). The sensing material was characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM). Electro-kinetic parameters such as heterogeneous rate constant, transfer coefficient, activation energy, and the number of protons and electrons involved in the reduction of ACF have been determined. The SWV technique was employed to detect ACF at trace level concentration. Linearity was observed over the range of 0.1 mM-0.8 mM with a limit of detection at 1.28 nM of the analyte. Biological, agricultural and environmental relevance of the method developed was successfully applied to the monitoring of ACF in wastewater as well as in actual soil samples.

### **IP-06: Calcium-doped Zinc Oxide Nano Sensor for the Electrochemical Analysis of Algaecide Dichlone**

**Davalasab Ilager and Nagaraj P. Shetti\***

*Department of Chemistry, KSS Art's, Science & Commerce College and PG Centre, Gadag - 582101, Karnataka  
E-mail : davalasabilager@gmail.com*

The voltammetric sensor incorporated with synthesized calcium-doped zinc oxide (Ca-ZnO/CPE). The cyclic voltammetry (CV) method was employed to determine the electrochemical behavior of dichlone



(DCN), referred to as fungicide and algaecide. The surface morphology of the developed sensor's matrix was carried out employing SEM, TEM, and XRD techniques. The Ca-ZnO NPs as a modifier in the carbon paste efficiently enhanced both the oxidative and reduction peak current of DCN in CVs. The effect of electrolyte pH and scan rate variation investigation results were used to determine the total number of electrons in the DCN electro-oxidation mechanism, the number of protons, charge transfer coefficient, and heterogeneous rate constant. The square wave voltammetry technique (SWV) showed the lowest detection limit (DL) of  $5.98 \times 10^{-8}$  M and a wide linearity range ( $3.5 \times 10^{-7}$  M to  $7.2 \times 10^{-4}$  M). The environmentally-based approach successfully quantifies DCN in water and soil samples.

### **IP-07: Three Isomeric New Bismuth(III) Dithiocarbamates as Anticancer Agents: Synthesis, Structure and Cytotoxicity**

**Deepika Verma and Om Prakash\***

*Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow-226007, U.P.*

*E-mail : prakash\_om@lkouniv.ac.in; ops92002@gmail.com*

Metal anticancer agents are expanding beyond Pt drugs. Here we disclose three positional isomeric, homoleptic Bi(III) dithiocarbamates  $[\text{Bi}(\text{S}_2\text{C}-\text{N}(\text{CH}_2\text{Ph})(\text{CH}_2-\text{X}-\text{HO}-\text{C}_6\text{H}_4))_3]$  (X=2,3,4 Bi-2ba, Bi-3ba, and Bi-4ba, respectively) named as tris[(N-benzyl-N-(X-hydroxybenzyl) dithiocarbamato- $\kappa^2\text{S,S}$ )] bismuth (III). IR,  $^1\text{H}/^{13}\text{C}\{^1\text{H}\}$  NMR, UV-vis and HRMS support  $\kappa^2(\text{S,S})$  chelation of three DTC ligands at Bi (III). DFT indicates the isomers are essentially isostructural, giving a distorted pseudo-octahedral S6 environment (Bi-S 2.76–2.84 Å; bite S–Bi–S  $\approx 84^\circ$ ; thioureide N–C  $\approx 1.34$ – $1.35$  Å). In A549 cells (MTT, 24 h) potency follows Bi-4ba ( $\text{IC}_{50} \approx 10 \mu\text{M}$ ) > Bi-3ba ( $\approx 20 \mu\text{M}$ ) > Bi-2ba ( $\approx 60 \mu\text{M}$ ); 5-fluorouracil (5-FU)  $\approx 20 \mu\text{M}$  under identical conditions. Mechanistic assays, including ROS, JC-1/MitoTracker, and DAPI staining, reveal pronounced intracellular ROS generation accompanied by mitochondrial membrane depolarization, consistent with oxidative and mitochondria-mediated stress pathways; docking suggests engagement of apoptosis-related proteins (e.g., caspase-3/caspase-9, BCL-2/BCL-XL). Swiss ADME flags the Bi complexes as large, lipophilic, and poorly soluble with low predicted GI absorption (vs drug-like, highly soluble 5-FU). These results identify Bi-aryl-DTC scaffolds as tunable, non-platinum anticancer candidates with a ROS/mitochondria-centred mode of action.

## **IP-08: Design and Construction of Quinoline based Rhodium(III) Organometallic Complex: Catalytic Utility in the Synthesis of Succinimides Containing Late-Stage Drug Candidates**

**Tanya Tripathi<sup>1</sup>, Neeraj Kumar Mishra<sup>1\*</sup> and In Su Kim<sup>2\*</sup>**

<sup>1</sup>Department of Chemistry, University of Lucknow, Lucknow - 226007, U.P.

<sup>2</sup>School of Pharmacy, Sungkyunkwan University, Suwon -16419, Republic of Korea

E-mail : neerajchemistry@gmail.com<sup>1\*</sup>; insukim@skku.edu<sup>2\*</sup>

Cyclometalated rhodium complexes constitute an important class of organometallic chemistry. Although such compounds are well documented in the literature, rhodium(III) cyclometalates are an important complex plays a crucial role in cross coupling reactions. In this addition, the design and synthesis of in situ generated quinoline based organometallic rhodium(III)-complex was found to be more reactive catalytic complex in various cross-coupling reactions. Moreover, from last few years, in situ generated Rh(III) complex has been efficiently utilized in the formation of various heterocycles. In continuation to this, Mishra and Kim et. al. successfully reported a range of work by using the in situ generated Rh(III) complex for late-stage heterocycles<sup>1</sup>. In this context, the construction of a quinoline-based Rh(III) organometallic complex obtained from [RhCp\*Cl<sub>2</sub>]<sub>2</sub> and investigate its catalytic utility in the construction of succinimide containing drug molecules.

This newly synthesized complex, characterized by NMR, UV-Vis, and IR spectroscopy, shows a Cp\*Rh(III) core that shows high stability and facilitates effective reaction. Owing to its catalytic potential, the synthesized activated Rh(III) complex was efficiently applied to quinoline for the incorporation of succinimides at C7 position of quinoline moieties and delivered a range of late-stage drug candidates in combination of two drug candidates, which I will explain during my poster presentation.

## **IP-09: Tuning Heterogeneous OER Electrocatalytic Activity in Ni(II)-tris-(2-aminoethylamine) Dithiolates through -OMe Positional Isomerism**

**Shreya Srivastava, Aparna Kushwaha, Madhav Raj Jayswal and Abhinav Kumar\***

Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow - 226 007

E-mail : abhinavmarshal@gmail.com; kumar\_abhinav@lkouniv.ac.in

Rational tailoring of ligand architectures, especially via positional isomerism of judiciously selected functional groups, can effectively

tune the metal-centered electronic environment and consequently elevate the electrocatalytic activity of the resulting coordination complexes. Three new positional isomeric -OMe based heteroleptic Ni(II) dithiolates appended with tris-(2-aminoethyl amine) (tetraen) co-ligand having compositions [Ni(S<sub>2</sub>C(CN)(o-OMeC<sub>6</sub>H<sub>5</sub>)(tetraen)] (o-Ni-OMe), [Ni(S<sub>2</sub>C(CN)(m-OMeC<sub>6</sub>H<sub>5</sub>)(tetraen)] (m-Ni-OMe) and [Ni(S<sub>2</sub>C(CN)(p-OMeC<sub>6</sub>H<sub>5</sub>)(tetraen)] (p-Ni-OMe) have been synthesized and characterized. The complexes possess distorted octahedral geometries around Ni(II) where it is coordinated with two sulfur of the dithiolate ligand and four nitrogen atom of the tetraen ligand. The complexes have been used as heterogeneous molecular electrocatalysts for oxygen evolution reaction (OER) under alkaline conditions. The results suggest the best electrocatalytic performance of m-Ni-OMe with  $\eta^{10}$  of 448 mV and small Tafel slope of 68.7 mV·dec<sup>-1</sup>. The study suggests that the electrocatalytic performance is governed by the Hammett electronic effect of the -OMe substituent and the dihedral angle between the NiS<sub>2</sub>C<sub>2</sub> plane and the aromatic ring, which together modulate electron density and optimize orbital overlap during OER. The study shows the synergistic interplay of substituent electronic effect and molecular framework Ni–dithiolate electrocatalysts with enhanced oxygen evolution efficiency.

### **IP-10: Strategic Design of Ni(II)-Dithiolate-1,10-Phenanthroline Complexes: Influence of Isomeric Methoxy Substitutions on Dihedral Angle-Hammett Interplay on Oxygen Evolution Reaction Performance**

**Madhav Raj Jayswal, Daniel Omoding, Shreya Srivastava, Aparna Kushwaha and Abhinav Kumar\***

*Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow - 226007*

*E-mail : kumar\_abhinav@lkouniv.ac.in; abhinavmarshal@gmail.com*

The three new heteroleptic 1,10-phenanthroline (Phen) appended Ni(II) complexes bearing positional isomeric methoxyphenyl-acetonitriledithiolates [Ni(L1)Phen] (2Ni-Phen), [Ni(L2)Phen] (3Ni-Phen), and [Ni(L3)Phen] (4Ni-Phen) (L1 = disodium 2-methoxyphenylacetonitriledithiolate; L2 = disodium 3-methoxyphenylacetonitriledithiolate; L3 = disodium 4-methoxyphenylacetonitriledithiolate) have been synthesized and characterized. Gas-phase geometry optimization reveals distorted square-planar coordination around Ni(II). The electrocatalytic activity trends are strongly governed by both the Hammett electronic effect of the methoxy substituent and the dihedral angle between the NiS, C, plane and the appended aromatic ring. Among them, 3Ni-Phen displays the best OER performance with

an onset potential of 1.56 V (vs. RHE),  $\eta^0$  of 327 mV,  $\eta^5$  of 385 mV,  $\eta^{10}$  of 410 mV, highest turnover frequency of  $284.468 \times 10^{-3} \text{ s}^{-1}$  at  $\eta = 750$ , and a remarkably low Tafel slope of  $53 \text{ mV} \cdot \text{dec}^{-1}$ . Post-OER FESEM analysis further confirms the retention of nanoscale morphological features in 3Ni-Phen relative to significant surface coarsening in 2Ni-Phen and 4Ni-Phen, underpinning its enhanced structural robustness and sustained activity. This study demonstrates that the synergistic interplay of substituent electronic effects, coordination dihedral angle, and morphological stability provides a rational framework for designing Ni-dithiolate molecular electrocatalysts for efficient oxygen evolution.

## **IP-11: Fabrication of MnO<sub>2</sub> Nanoparticle-Modified Electrode for Sensitive and Selective Detection of Valaciclovir**

**Pruthvi G. Sajjannavar and Jayant I. Gowda\***

*Department of Chemistry, BLDEA's Commerce, B.H.S. Arts and T.G.P. Science College, Jamkhandi - 587301, Karnataka*

*Research Centre in Chemistry, BLDEA's Commerce, B.H.S. Arts and T.G.P. Science College, Affiliated to Bagalkot University, Jamkhandi - 587301, Karnataka*

*E-mail : jayantgowda4@gmail.com*

The electrochemical investigation of valaciclovir (VAL) was performed using a glassy carbon electrode modified with electro-deposited manganese oxide nanoparticles (MnO<sub>2</sub>/GCE). The surface morphology of the fabricated sensor material was characterized through scanning electron microscopy (SEM). The influence of scan rate, solution pH, and analyte concentration on the electrochemical response of VAL was systematically examined using cyclic voltammetry (CV) and differential pulse voltammetry (DPV). A significant enhancement in anodic peak current was observed for the modified electrode (5.76  $\mu\text{A}$ ) compared to the bare GCE (1.18  $\mu\text{A}$ ), demonstrating the improved surface area and catalytic efficiency of the manganese oxide nanoparticles. The DPV results exhibited a linear relationship between peak current and VAL concentration within the range of  $1.0 \times 10^{-8} \text{ M}$  to  $1.4 \times 10^{-5} \text{ M}$ . The calculated limits of detection (LOD) and quantification (LOQ) were 0.95 nM and 3.17 nM, respectively. The sensor's practical applicability was confirmed through successful determination of VAL in pharmaceutical formulations and real samples. These findings suggest that the developed electrochemical sensor possesses excellent potential for use in quality control laboratories for pharmaceutical analysis.

## IP-12: Tertiary Phosphane-Modified Ni(II) 1,3-Benzothiazol-2-ylacetoneitriledithiolates: Tuning Heterogeneous OER Electrocatalysis through Phosphane Denticity, Steric Modulation, and Chelate Ring-size Variation

Daniel Omoding<sup>1</sup>, Madhav Raj Jayswal<sup>1</sup>, Gabriele Kociok-Köhn<sup>2</sup> and Abhinav Kumar<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow 226007

<sup>2</sup>Physical Structure Characterization, University of Bath, Claverton Down, Bath, BA2 7AY, UK

E-mail : abhinavmarshal@gmail.com

Developing active and stable transition metal electrocatalysts for oxygen evolution reaction is essential for many renewable energy conversion processes. Herein, three new heteroleptic Ni(II)-dithiolates viz. [(Bzdt)Ni(PPh<sub>3</sub>)<sub>2</sub>], [(Bzdt)Ni(dppe)] and [(Bzdt)Ni(dppf)] (Bzdt<sup>2-</sup> = 1,3-benzothiazol-2-ylacetoneitriledithiolate, PPh<sub>3</sub> = triphenylphosphine, dppe = 1,2-bis(diphenylphosphino)ethane and dppf = 1,1'-bis(diphenylphosphino)ferrocene) have been synthesized, and their molecular structures were elucidated by various spectroscopic methods, FESEM-EDS and in one case, [(Bzdt)Ni(dppe)] by SCXRD. In [(Bzdt)Ni(dppe)], the Ni(II) core adopts a distorted square planar geometry that is satisfied by two S atoms and two P atoms of corresponding bzdt<sup>2-</sup> and dppe ligands, and its Hirshfeld surface analyses revealed existence of C-H...S, C-H...Ni, C-H...N, and C-H...C non-covalent interactions, that sustained its supramolecular architecture. All complexes exhibited significant activities towards OER in basic media (current density,  $j > 46.11 \text{ mA.cm}^{-2}$ ) at  $10 \text{ mV} \cdot \text{s}^{-1}$ , with a dppe appended Ni(II)-dithiolate complex, [(Bzdt)Ni(dppe)] demonstrating the best performance among the three, since it delivered a  $j$  value of  $10 \text{ mA.cm}^{-2}$  at a least overpotential of 354 mV and Tafel slope of  $53 \text{ mV.dec}^{-1}$ . The best activity observed with [(Bzdt)Ni(dppe)] is attributed to low charge-transfer resistance and band gap which facilitates electron transfer processes that are crucial for electrocatalysis.

## IP-13: Nano-Flake-Like ZnO-doped Structure for Electrochemical Activity as a Sensor for the Detection of Mefenamic Acid

Tarun K.<sup>1</sup>, Ronald Mascarenhas<sup>1</sup>, Shikandar D. Bukkitgar<sup>2</sup> and Nagaraj P. Shetti<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, St. Joseph's University, Lalbagh Road, Bengaluru - 560027 Karnataka

<sup>2</sup>Centre for Energy and Environment, School of Advanced Sciences, KLE

The present work demonstrates a simple co-precipitation method for synthesizing ZnO nanoparticles doped with 10% Magnesium. The morphological characteristics of doped ZnO nanoparticles were utilized to develop an electrochemical sensor. The structural investigation with XRD suggested the crystalline, hexagonal wurtzite structure. The EDX revealed the elemental composition of the synthesized material. Moreover, the SEM images confirmed the nanoflake-like structures. Furthermore, the synthesized material was utilized to construct an electrochemical sensor for detecting mefenamic acid. The modification of the carbon matrix with a nanostructure enhanced the surface-to-volume ratio, thereby enhancing the electro-catalytic activity of the sensor. The significant observations included a low limit of detection, good recoveries from the sample, and high stability, making it a suitable alternative for clinical trials.

### **IP-14: Bioengineered Fe/Ni-Lignin Composite Adsorbents Derived from Agri-Waste for the Removal of Emerging Pollutants**

**Megha M. Karki<sup>1</sup>, Santosh K.N.<sup>2</sup>, Shilpa S.H.<sup>1</sup> and S.K. Nataraj<sup>2</sup>**

<sup>1</sup>*KLE Society's Raja Lakhamagouda Science institute (Autonomous), Belagavi, Karnataka*

<sup>2</sup>*Centre for Nano & Material science, Jain Global Campus, Jain University, Jakkasandra Post, Ramanagara, Bangalore - 562112, Karnataka*  
*E-mail : sk.nataraj@jainuniversity.ac.in.*

Pharmaceutical and food additive contaminants such as tartrazene persist in aquatic environments, causing ecological and health concerns. In this study, an Fe–Ni lignin composite was synthesized from areca husk lignin via chemical precipitation using FeCl<sub>3</sub> and NiCl<sub>2</sub>. The composite was characterized using FTIR, DLS, and zeta potential analysis. Zeta potential measurements revealed a positively charged surface favorable for anionic dye adsorption, while DLS indicated a particle size distribution in the nanometer range, enhancing dispersion and reactivity. FTIR confirmed successful metal incorporation and functional group involvement in adsorption. Batch adsorption experiments showed high tartrazene removal efficiency under optimized pH and contact time, with adsorption following the (Langmuir/ Freundlich) isotherm model. The findings demonstrate the potential of Fe–Ni lignin composites as low-cost, sustainable adsorbents for targeted removal of anionic pollutants from wastewater.

## **IP-15: Comparing Fluoro- and Trifluoromethyl-Functionalized Ni(II) 1,1-dithiolates with 1,12 -bis-(diphenylphosphino)ferrocene co-ligand in DSSC Applications**

**Aparna Kushwaha, Devyani Srivastava and Abhinav Kumar\***

*Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow - 226 007*

*E-mail : abhinavmarshal@gmail.com*

A typical DSSC setup involves a photo-anode with a light harvester on a semiconducting material (such as nanocrystalline  $\text{TiO}_2$ ), a counter electrode, and a redox mediator. Four new heteroleptic Ni(II)-dithiolates with general formula  $[\text{Ni}(\text{dppf})(\text{dithiolate})]$  (dithiolate = 2-cyano-2-(4-fluorophenyl)ethene-1,1-bis(dithiolate) (Ni-1); 2-cyano-2-(2-(trifluoromethyl)phenyl)ethene-1,1-bis(thiolate) (Ni-2); 2-cyano-2-(3-(trifluoromethyl)phenyl)ethene-1,1-bis(thiolate) (Ni-3) and 2-cyano-2-(4-(trifluoromethyl)phenyl)ethene-1,1-bis(thiolate) (Ni-4); dppf = 1,12 -bis(diphenylphosphino) ferrocene) have been synthesized and characterized spectroscopically as well as by single crystal X-ray diffraction technique. Single crystal X-ray analyses for Ni-1 and Ni-2 reveal distorted square planar geometry around Ni(II) that are satisfied by two sulfur and two phosphorus centers of the dithiolate and dppf ligands, respectively. These complexes have been used as photosensitizers in  $\text{TiO}_2$ -based dye-sensitized solar cells (DSSCs) which suggest that the performance of fluoro-substituted sensitizer Ni-1 is superior to that of the other three trifluoromethyl-substituted sensitizers. Ni-1 showcases an efficiency ( $\eta$ ) of 5.47/ %, open circuit potential ( $V_{\text{oc}}$ ) of 0.699/ V, short circuit current ( $J_{\text{sc}}$ ) of 12.17/  $\text{mA cm}^{-2}$  and display 64/ % incident photon-to-current conversion efficiency. The plausible reason for the variation in photovoltaic performances have been explained by integrated experimental methods and theoretical calculations. Results indicate that the small sized fluoro-group exhibits significant p-orbital overlap with the aromatic fragment of the dithiolate ligand thereby enhancing the electron donation from  $\text{dppf} \rightarrow \text{Ni(II)} \rightarrow \text{dithiolate}$ .

## **IP-16: Two-Dimensional Bimetallic Fe-Mn Metal-Organic Framework (MOF)- $\text{MoS}_2$ based Nano Sheets for Effective Adsorption of Water Soluble Organic Contaminants**

**Rohini V Latkar, Ashok Shrishail Maraddi, Dibyendu Mondal\* and S.K. Nataraj\***

*Sustainable Energy Materials and Processes Research Group, Centre for Nano & Material Sciences, JAIN University, Jain Global Campus, Bangalore-562112*



Effective remediation of organic and inorganic pollutants from industrial wastewater is vital for achieving environmental sustainability. In this study, a novel two-dimensional bimetallic Fe–Mn metal–organic framework (MOF) integrated with MoS<sub>2</sub> nanosheets was engineered through a solvothermal route for the efficient adsorption and removal of water-soluble contaminants, including Congo Red, Methyl Orange, CrO<sub>4</sub><sup>2-</sup>, and Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup>. The synergistic redox interaction between Fe and Mn centers enhances adsorption affinity and oxidative potential, while MoS<sub>2</sub> nanosheets contribute a high specific surface area, abundant active sites, and superior electron transport. Composites with varying FeMn–MOF with MoS<sub>2</sub> molar ratios (1:1, 1:2, and 2:1) were synthesized and characterized using FTIR, XRD, FESEM, TGA, and zeta potential analyses. Among these, the FeMn–MOF–MoS<sub>2</sub> (2:1) hybrid exhibited the highest adsorption performance, showing excellent affinity toward CrO<sub>4</sub><sup>2-</sup>, Congo red, Methyl Orange, and Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup>. Continuous flow filtration experiments demonstrated its outstanding adsorption capacity, enhanced selectivity for anionic pollutants, and stable permeability. Kinetic studies confirmed a pseudo-second-order adsorption behavior, indicating chemisorptive interaction. In large-scale filtration, the FeMn–MOF–MoS<sub>2</sub> (2:1) composite effectively treated up to 1 L of Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup>-laden wastewater and retained above 98% efficiency after ten reuse cycles for conged red dye. These findings highlight the potential of Fe–Mn MOF–MoS<sub>2</sub> composites as durable, selective, and high-performance adsorptive membranes for advanced wastewater treatment.

### **IP-17: Coordination Behavior and Structure–Activity Relationship of A Quinoline-Based Oxime Ligand (LH) and Its Transition Metal Complex**

**Ganesh S. Hegde<sup>1</sup> and Vidyanand K. Revankar<sup>2\*</sup>**

<sup>1</sup>*Department of Chemistry, M. E. S., M. M. Arts & Science College, Sirsi - 581402, Karnataka*

<sup>2</sup>*Department of Chemistry, Karnatak University, Pavatenagar, Dharwad - 580003, Karnataka*

*E-mail : ganeshwinu16@gmail.com; vkrevankar@rediffmail.com*

The oxime-derived quinoline ligand 2-oxo-1,2-dihydro-quinoline-3-carbaldehyde oxime (LH) and its Co(II), Ni(II), Cu(II) and Zn(II) complexes were synthesized and characterized to assess their structural, spectroscopic and antimicrobial properties. LH was obtained in good yield and single crystals suitable for X-ray diffraction were grown; the ligand crystallizes in the quinolone (keto) tautomeric form and features an intramolecular O–H···O=C hydrogen bond. Reaction of LH with M(II) salts afforded stable solids assigned as [Co(LH)(L)Cl(H,

O)] (C1),  $[\text{Ni}_2(\text{L})_2\text{Cl}_2(\text{H}_2\text{O})_2]$  (C2),  $[\text{Cu}_2(\text{LH})(\text{L})\text{Cl}_2(\text{H}_2\text{O})_2(\mu\text{-Cl})_2]$  (C3) and  $[\text{Zn}(\text{LH})_2\text{Cl}_2]$  (C4) on the basis of elemental analysis, ESI-MS and CHN data. IR,  $^1\text{H}$  /  $^{13}\text{C}$  NMR (Zn-derivatives), and electronic spectra support bidentate coordination of LH via quinoline-carbonyl-O and azomethine-N, with evidence for enolization/deprotonation in selected complexes (notably the Ni derivative). Electronic and EPR data indicate distorted octahedral or elongated geometries for several species (C3 shows  $\text{dx}^2\text{-y}^2$  ground-state features). Thermal analyses reveal appreciable thermal stability up to  $\sim 250\text{--}300^\circ\text{C}$  depending on the complex. Notably, LH and its metal complexes display potent antibacterial activity (MICs down to  $0.4\ \mu\text{g}\cdot\text{mL}^{-1}$  against *Staphylococcus aureus* and *Escherichia coli*), markedly surpassing the ciprofloxacin control ( $2\ \mu\text{g}\cdot\text{mL}^{-1}$ ). These combined structural and bioactivity results nominate the LH-M(II) series as promising scaffolds for further antimicrobial development.

### **IP-18: Synthesis, Characterization of Schiff Bases Derived Chromium(III) and Manganese(III) Complexes with 5-substituted Isatin and 4-substituted Thiosemicarbazides**

**V. K. Sharma<sup>1\*</sup> and Vinay Kumar Gupta<sup>2</sup>**

<sup>1</sup>*Department of Chemistry, University of Lucknow, Lucknow - 226007 (U.P.)*

<sup>2</sup>*School of Basic Sciences, Babu Banarasi Das University, Lucknow - 226028 (U.P.)*

*E-mail : vinaygupta1240@bbdu.ac.in; vksharma21@hotmail.com*

The new Chromium(III) and Manganese(III) complexes of the general formula  $[\text{M}(\text{LH})_2]\text{Cl}$  (M=Cr(III) and Mn(III); LH = Schiff bases derived from Isatin / 5-Chloroisatin / 5-Bromoisatin / 5-Flouroisatin / 5-Nitroisatin and 4-Methyl-3-thiosemicarbazide / 4-Phenyl-3-thiosemicarbazide) have been prepared. As an extension of our studies on both the coordination chemistry of heteroatom containing ligands and on the catalytically application of their metal complexes, we report the synthesis of a series of new chromium(III) and manganese(III) complexes containing bidentate Schiff base ligands. Schiff bases and their metal complexes are increasingly being used as catalysts in various biological systems, polymers and dyes. Moreover, it is confirmed that these compounds can act as enzyme preparations. The complexes have been characterized by elemental analysis, electrical conductance, magnetic moment and spectral (electronic, infrared) data. The complexes exhibit octahedral geometry around metal center. The ligand and all compounds were assayed for antibacterial (*Bacillus Pumilus* and *Escherichia Coli*) and antifungal (*A. niger* and *C. albicans*) activities. The activities have been correlated with structures of compounds. The metal chelates had more antifungal activity than the uncomplexed Schiff bases.

## IP-19: Experimental and Computational Analysis of Quinoline-Schiff Base Transition Metal complexes with dual Antimicrobial and antioxidant Activities

Sulochana P. Melinmath<sup>1\*</sup>, Venkatesh K. Bhovi<sup>2\*</sup> and Venkatesh T.<sup>3</sup>

<sup>1</sup>Department of Chemistry, Kishkinda University, Mountview Campus, Ballari-583104

<sup>2</sup>Department of Chemistry, Vijayanagar College, Hosapete Vijayanagar-583201

<sup>3</sup>Department Chemistry, Kuvempu University, Shankaraghatta-577451

E-mail : sulochanapm2@gmail.com

This study reports the design, synthesis, and multi-faceted evaluation of novel Schiff base ligand N-((2-chloro-6-methylquinolin-3-yl)methylene)quinoline-2-carbohydrazide (L), and its metal complexes (Cu(II), Co(II), Ni(II), Zn(II)) (4a-d). The ligand was synthesized by the condensation of Quinoline-2-carbohydrazide (QCH) with 2-chloro-6-methylquinoline-3-carbaldehyde (2C3FQ). The synthesized metal complexes were characterized by elemental analysis, FTIR, NMR, Mass spectra, molar conductance and magnetic measurements. The analytical data reveals that ligand acts as bidentate ligand and forms complex of (M-L)1:1 stoichiometry with octahedral geometry. The biological profile of the compounds was extensively investigated. The metal complexes demonstrated significantly enhanced bioactivity compared to the free ligand. Particularly, the [Co(L)(H<sub>2</sub>O)<sub>3</sub>Cl] and [Cu(L)(H<sub>2</sub>O)<sub>3</sub>Cl] complexes exhibited superior antimicrobial potency than the other metal complexes. The antioxidant studies revealed exceptional, radical-specific scavenging efficacy: the [Cu(L)(H<sub>2</sub>O)<sub>3</sub>Cl] complex was most potent in the DPPH assay, while the [Co(L)(H<sub>2</sub>O)<sub>3</sub>Cl] complex excelled in nitric oxide radical scavenging and ferrous ion chelation assay. Assay of PLA<sub>2</sub> by indirect hemolytic activity showed complexes (4a, 4d) along with the ligand inhibited the activity of russel viper venom suggesting promising antivenom applications. Complementing the experimental data, DFT calculation provides the theoretical insights into the electronic properties, including HOMO-LUMO energy bandgap and dipole moments, correlating stability and reactivity with the observed biological trends. These results collectively position these complexes, particularly those of Cu(II) and Co(II), as highly promising candidates for therapeutic development, spanning as antimicrobial and antioxidant agents.

## **IP-20: Pd-catalyzed Synthesis of Benzoxazolone Derivatives and In-silico Study Targeted TSPO Protein for Neuro-inflammation Treatment**

**Nidhi, Khushboo Singh and Vinay Kumar Singh\***

*Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow-226007, U.P.*

*\*E-mail : vinayksingh.lu@gmail.com; nidhichemistry27@gmail.com*

Benzoxazolones are multifaceted heterocyclic structures recognized for their diverse range of biological effects, such as anti-inflammatory, antimicrobial, and anticancer properties. In this study, we established an effective palladium-catalyzed carbonylative cyclization approach for the creation of substituted 2(3H)-benzoxazolones utilizing o-haloanilines and o-aminophenols. The reaction occurs under mild conditions with the use of Pd(OAc)<sub>2</sub> and phosphine ligands alongside CO, resulting in the desired heterocycles being produced in good to excellent yields. This method demonstrates a wide range of substrate applicability, tolerance of various functional groups, and ease of operation, thus making it ideal for the quick synthesis of bioactive analogs. Translocator Protein (TSPO, 18kDa) is found throughout the outer mitochondrial membrane and is notably abundant during the activation of microglia in neuroinflammatory disorders. The translocator protein (TSPO, 18kDa) serves as a highly valuable biomarker for investigating the impact of neuroinflammation in both humans and different animal species. In-silico analyses of synthesized benzoxazolone derivatives indicated strong interactions with translocator proteins. These results imply that benzoxazolone derivatives could serve as a potential marker for the visualization of neuroinflammation through targeting TSPO.

## **IP-21: Rare Metal Complexes with N,O-Donor Benzimidazole Ligands: Spectroscopic Characterization and Functional Applications**

**Haresh R. Patel**

*Department of Chemistry, Khedbrahma Campus, HNGU, Vadali*

*E-mail : hareshpatel6900@yahoo.com*

Heterocyclic compounds are widely present in natural products such as carbohydrates, amino acids, vitamins, alkaloids, and glycosides, and they play an important role in pharmacological activity. Benzimidazole derivatives, in particular, are of great interest due to their biological potential. In this work, a new derivative of 2 mercapto 5 methoxybenzimidazole was synthesized by linking it with N-(4-acetylphenyl)-2-chloroacetamide. Preliminary studies were also conducted to investigate its biological activities and catalytic properties. The results suggest that such modified Benzimidazole derivatives may serve as promising candidates for medicinal and industrial applications.

## **IP-22: Carbon Paste Electrode Sensor for EBT using Copper Oxide Nanoparticles**

**Rajeshwari Yemmi and B.E. Kumara Swamy\***

*Department of PG Studies and Research in Industrial Chemistry, Kuvempu University, Jnana Sahyadri Shankaraghatta - 577451, Shivamogga, Karnataka  
E-mail : kumaraswamy21@gmail.com*

In the present study, copper oxide nanoparticles (CuO/NPs) were prepared using coprecipitation method and then examined using scanning electron microscopy, X-ray diffraction and energy dispersive spectroscopy techniques. Synthesized CuO/NPs were subjected to antibacterial activity against evaluated disruptive bacterial strains, and the results demonstrate a strong, considerable zone of inhibition. Using cyclic voltammetry approach, carbon paste electrode modified by CuO/NPs was utilized for further detailed electro-analysis of Eriochrome Black T (EBT). At modified carbon paste electrode, effective electrocatalytic activity for the reduction of EBT was demonstrated. It was observed that the obtained LOD values for two reduction peaks of EBT are 42.2  $\mu\text{M}$  and 109.9  $\mu\text{M}$ , while LOQ values are 140.7  $\mu\text{M}$ , and 366  $\mu\text{M}$ , respectively. It was determined that modified electrode shows achieved reusability, stability and reproducibility as well as it shows good interference with other interfering compounds.

## **IP-23: Dihydroxy Benzene Isomers at Clayton Yellow Modified Carbon Paste Electrode**

**Chethan M Kuskur and B.E. Kumara Swamy\***

*Department of P.G. Studies and Research in Industrial Chemistry, Kuvempu University, Jnana Sahyadri, Shankargatta, Shimoga - 577451, Karnataka  
E-mail : kumaraswamy21@yahoo.com*

In order to detect 1, 2-dihydroxybenzene (CA) and 1, 4-dihydroxybenzene (HY), a small, sensitive, and effective chemically modified electrode was developed by electrochemically polymerizing Clayton yellow (CY) modified carbon paste electrodes (Clayton Yellow/MCPE) with NaOH (0.1mM) as a supporting electrolyte. An electro-oxidation of CA and HY using the fabricated film-coated electrode showed excellent electrocatalytic performance. A sweep rate investigation was carried out to determine the electrode process kinetics and the results confirm the diffusion-controlled. A pH analysis showed that proton and electron transfers were equal in number, and that redox potentials were pH-dependent. The concentration investigations indicated that the detection limits for CA and HY are 2.0 and 2.7, respectively. Additionally, phenolic isomers were successfully separated in a binary mixture. Tap water sample analysis was performed to assess the analytical performance of the Clayton Yellow/MCPE and positive recovery outcomes were obtained.

## **IP-24: Enzyme-Immobilized Metal–Organic Frameworks: Advances in Biosensing, Biocatalysis, Drug Delivery and Cancer Therapy**

**Deepika Verma and Om Prakash\***

*Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow - 226007, U.P.*

*E-mail : prakash\_om@lkouniv.ac.in; ops92002@gmail.com*

Enzymes play a vital role in catalysis, biosensing, and therapeutic processes, yet their instability under harsh reaction or physiological conditions limits practical applications. Metal–organic frameworks (MOFs), characterized by their high porosity, tunable structure, and chemical robustness, provide an ideal platform for enzyme immobilization. Immobilizing enzymes within MOFs enhances their operational stability, activity retention, and recyclability, overcoming the constraints of free enzymes. The resulting enzyme–MOF composites exhibit remarkable performance across multiple domains—biosensing, biocatalysis, targeted drug delivery, and cancer therapy. In biomedical applications, these hybrids enable site-specific drug release and improved bioavailability, reducing off-target effects during cancer treatment. Their integration into biosensing systems facilitates rapid, sensitive, and selective detection of biomarkers, aiding in early diagnosis and disease monitoring. Moreover, in biocatalysis, enzyme-MOFs promote sustainable and efficient transformations relevant to green chemistry, pharmaceuticals, and biofuel production. This review critically discusses enzyme immobilization strategies, structural–functional relationships, and emerging biomedical applications of enzyme-MOFs, while highlighting current challenges and future prospects for advancing multifunctional bio-hybrid materials.

## **IP-25: Green Synthesis of Zinc Oxide Nanostructures by Cymbopogon Citratus and Investigation of Surface Modification by 2-aminothiophenol on Optoelectronics Properties**

**Parappa Koshti<sup>1</sup>, Mallikarjunagouda B. Patil<sup>1\*</sup> and Ravi C. Bharamagoudar<sup>2</sup>**

*<sup>1</sup>Bharat Ratna Prof. CNR Rao Research Centre, Basaveshwar Science College, Bagalkot-587101, Karnataka*

*<sup>2</sup>Department of Physics, Jain College of Engineering, Belagavi, Karnataka  
E-mail : mallupatil04@gmail.com*

This study describes a green synthesis of ZnO nanoparticles using a precipitation method with cymbopogon citratus (lemongrass) as the natural precursor. To prevent agglomeration, 2-aminothiophenol was used as a capping agent, allowing for effective surface modification of



the ZnO nanostructures. The optoelectronic properties of the synthesized nanoparticles were thoroughly investigated, with a focus on the effect of 2-aminothiophenol capping using fluorescence and UV-visible (UV-vis) spectroscopy. The findings show that surface capping significantly alters the optical behavior of ZnO nanoparticles, reducing visible emission from surface defects while increasing UV emission. The absorption spectra showed a blue shift in the absorption edge, indicating that the electronic properties had changed due to surface passivation. These findings suggest that 2-aminothiophenol effectively passivates surface defects, improving ZnO's optoelectronic performance. Surface area analysis and NH<sub>3</sub>-TPD studies showed that green-synthesized, modified ZnO has superior structural and surface properties than neat ZnO. Electrochemical impedance spectroscopy (EIS) revealed improved electrical conductivity in the modified ZnO nanoparticles. This study emphasizes the potential of surface-modified, green-synthesized ZnO for advanced optoelectronic applications, particularly UV laser technologies, by providing a sustainable and efficient method of tailoring its optical and electronic properties.

### **IP-26: Novel $\alpha$ , $\beta$ -diketo BF<sub>2</sub> Complexes for Strong Solid State Emission & Self Recovery Electrochromism**

**Yeshvanth S., Atul B. Nipate and Rajeswara Rao M.\***

*Department of Chemistry, Indian Institute of Technology Dharwad,*

*Dharwad – 580011, Karnataka*

*E-mail : cy24dp006@iitdh.ac.in*

Boron complexes have emerged as versatile functional materials due to their unique electronic properties and tunable coordination environments. Their ability to exhibit strong luminescence and redox activity makes them ideal for optoelectronic and other applications. This study shows a novel one step synthetic strategies for developing  $\alpha$ ,  $\beta$ -diaryl (1a) and  $\beta$ -diketo (3a) BF<sub>2</sub> Complexes.  $\alpha$ ,  $\beta$ -diaryl boron complexes fluorescence colour is tunned from cyan (470 nm) to Red (652 nm) with aggregation induced emission and  $\alpha$ -diketo boron complexes are dual state emissive, with  $\lambda_{\text{max}} = 525$  nm in solution state and  $\lambda_{\text{max}} = 600$  nm in solid state. These boron complexes were further extended with  $\pi$ -conjugation by Knoevenagel condensation with aromatic aldehyde 2a & 4a.  $\alpha$ ,  $\beta$ -diaryl boron complex are demonstrated for the electrochromism, which exhibits a drastic colour changes from colourless to purple upon applying a reduction potential of -1.3 V with spontaneous self-oxidation from the reduced state.



## **IP-27: Biological Potential of Heterocyclic Schiff base and their Transition Metal Complexes. “A Review”**

**Alok Kumar and Gayatri Kumari**

*Department of Chemistry, Saraswati Degree College, Hathras*

*E-mail: drgayatri.chem@gmail.com*

Heterocyclic Schiff bases and their transition metal complexes have received significant attention due to their versatile biological and pharmacological activities. Schiff bases, formed by the condensation of primary amines with carbonyl compounds, possess donor sites such as nitrogen, oxygen, and sulfur, which facilitate coordination with transition metals. These complexes often exhibit enhanced stability and bioactivity compared to the free ligands. Numerous studies reported that heterocyclic Schiff base metal complexes demonstrate promising antimicrobial properties against a broad spectrum of bacteria and fungi, attributed to improved lipophilicity, chelation, and ability to interact with biomolecules. This review summarizes recent advances in the synthesis, characterization, and antimicrobial evaluation of heterocyclic Schiff bases and their transition metal complexes, highlighting structure–activity relationships and potential applications in medicinal chemistry. The findings emphasize their role as promising candidates for the development of new antimicrobial agents in response to increasing drug resistance.

## **IP-28: Development of ZrO<sub>2</sub>-TiO<sub>2</sub> Binary Nanocomposites for Enhanced Energy Storage in Supercapacitors**

**Sridevi Patil<sup>1</sup>, Bipin S. Chikkatti<sup>1</sup>, Ashok M. Sajjan<sup>1,2\*</sup>  
and Nagaraj R. Banapurmath<sup>2</sup>**

*<sup>1</sup>Department of Chemistry, KLE Technological University, Hubballi 580031*

*<sup>2</sup>Centre of Excellence in Material Science, School of Mechanical Engineering,  
KLE Technological University, Hubballi - 580031*

*E-mail : am\_sajjan@kletech.ac.in; patilsripatil@gmail.com*

This study focuses on the development of ZrO<sub>2</sub>-TiO<sub>2</sub> binary nanocomposites for use in supercapacitor applications. The functionality of the nanoparticles is examined through Fourier transform infrared spectroscopy, X-ray diffraction while their surface morphology is analyzed using scanning electron microscopy. Electrochemical performance is evaluated using techniques such as Cyclic Voltammetry, Electrochemical Impedance Spectroscopy, and Galvanostatic Charge–Discharge measurements. The ZrO<sub>2</sub>/TiO<sub>2</sub> nanocomposite demonstrates a high specific capacitance of 226.5 F g<sup>−1</sup> at a current density of 0.75

A  $\text{g}^{-1}$ . It also exhibits impressive stability, retaining 86% of its capacitance and almost 100% coulombic efficiency after 4000 cycles. Moreover, the nanocomposite exhibits an impressive power density of  $5000 \text{ W kg}^{-1}$ , demonstrating its capability for rapid energy delivery, which is a critical requirement for high-power applications. Simultaneously, it achieves a high energy density of

$125.8 \text{ Wh kg}^{-1}$ , signifying its ability to store substantial amounts of energy per unit mass. Given these remarkable attributes, the  $\text{ZrO}_2\text{-TiO}_2$  nanocomposite emerges as a highly promising material for energy storage applications, offering a compelling alternative to conventional electrode materials and paving the way for the development of more efficient, sustainable, and high-performance electrochemical energy storage systems.

## **IP-29: Green Synthesis of Strontium substituted Barium Nanoferrites Using Lemon Extract via Modified Sol-Gel Auto-Combustion Method**

**Shridhar Mathad<sup>1\*</sup>, Sushant Kakati<sup>2</sup> and Maruti Rendale<sup>3</sup>**

<sup>1</sup>*Department of Engineering Physics, K.L.E Technological University, Vidyanagar, Hubballi*

<sup>2</sup>*Department of, East Point College of Engineering and Technology, Bangalore*

<sup>3</sup>*Department of Physics, KLS Gogte Institute of Techonlogy, Belagavi*

<sup>\*</sup>*E-mail : shridhar.mathad@kletech.ac.in*

This study explain a sustainable technique for preparing Sr doped Barium nanoferrites by employing the eco friendly method by modified sol-gel auto-combustion (MSG) process lemon extract as a natural fuel. This synthesis of ferrites may be done more environmentally friendly by using renewable resources, including fresh lemon extract that high in citric acid by avoiding traditional chemical processes. The organized nano ferrites were examined the usage of XRD (X-ray diffraction), FTIR (Fourier-transform infrared spectroscopy), SEM (scanning electronic microscopy) and VSM to get facts related to structural, morphological and magnetic characteristics. These findings reveal the advantageous alternative of  $\text{Sr}^{3+}$  ions into the Barium ferrite lattice, appreciably impacting the structural and magnetic characteristics. This work emphasizes how quintessential inexperienced synthesis methods are to growing trendy nano-materials that are used in electronics, biology, and magnetism.

## IP-30: Engineering Synergistic CuWO<sub>4</sub>NiS<sub>2</sub> Heterojunctions for High-Efficiency Photocatalytic Water Splitting

Risheek S. Hiremath<sup>1</sup>, Madasu Sreenivasulu<sup>2</sup>  
and Nagaraj P. Shetti<sup>2\*</sup>

<sup>1</sup>Department of Chemical Engineering, SRM University, Kattankulathur, Chennai, 603203, Tamil Nadu

<sup>2</sup>Centre for Energy and Environment, School of Advanced Sciences, KLE Technological University, Vidyanagar, Hubballi, 580 031, Karnataka  
E-mail : npshetti@kletech.ac.in

Photocatalytic hydrogen (H<sub>2</sub>) generation represents a promising and environmentally benign strategy for the production of green hydrogen. Nevertheless, the advance of efficient semiconductor materials that exhibit both high activity and long-term stability remains a significant challenge. In this study, we report the synthesis of a broadband-gap, UV light-responsive Cu-WO<sub>4</sub>/NiS<sub>2</sub> nanocomposite via a straightforward impregnation method. The photocatalytic presentation of the hybrid system was comprehensively evaluated using microscopic, spectroscopic, and photophysical characterization techniques. Under light irradiation, the optimized CuWO<sub>4</sub>/NiS<sub>2</sub> heterostructure achieved a remarkable H<sub>2</sub> evolution rate of 28.2 mmol h<sup>-1</sup> g<sup>-1</sup>, which is approximately 2.71 and 3.28 folds higher than that of pristine Cu-WO<sub>4</sub> (10.4 mmol h<sup>-1</sup> g<sup>-1</sup>) and NiS<sub>2</sub> (8.6 mmol h<sup>-1</sup> g<sup>-1</sup>), correspondingly. The improved presentation is attributed to the synergistic interaction between the coupled semiconductors, which facilitates the formation of a Type-II heterojunction. This configuration promotes effective charge carrier separation and suppresses electron-hole recombination. Moreover, the Cu-WO<sub>4</sub>/NiS<sub>2</sub> composite exhibited a significantly higher photocurrent density than that of pristine CuWO<sub>4</sub> and NiS<sub>2</sub>, respectively. This improvement is attributed to the increased density of catalytically energetic sites and the enhanced absorption of solar radiation. These findings highlight the considerable potential of CuWO<sub>4</sub>/NiS<sub>2</sub> as a noble-metal-free photocatalyst for sustainable hydrogen generation.

## IP-31: Selenium as An Efficient Pseudocapacitive Electrode Material for Supercapacitors

Shivakumar I. Mathapati, Darshana V. U and R. M. Hodlur\*

Department of Physics, School of Advanced Sciences, KLE Technological University, Hubballi – 580 031, Karnataka

E-mail: rm.hodlur@kletech.ac.in; shivurs007@gmail.com

Selenium (Se) has gained significant attention as an electrode material for supercapacitors due to its redox activity and high electrical conductivity. In this present work, elemental selenium was synthesized using the selenium dioxide (SeO<sub>2</sub>) as a precursor, and its crystalline

nature was confirmed by x-ray diffraction (XRD), which revealed characteristic peaks corresponding to trigonal Se. Selenium was further combined with graphene oxide (GO) and reduced graphene oxide (rGO) to form Se/GO and Se/rGO composites, respectively. Comparative electrochemical evaluation demonstrated that Se/rGO outperformed Se/GO, delivering a higher capacitance of 323 F/g at a scan rate of 5 mV/s with excellent rate capability, and superior cyclic stability, retaining 91% of its capacitance over 1000 cycles. The enhanced performance is attributed to the conductive rGO network, enabling more efficient charge storage. These findings indicate that Se/rGO is a promising electrode candidate for high performance supercapacitor electrodes.

### **IP-CYSA-01: Iron Oxide Magnetic Nanoparticles: A Boon for Pharmaceutical Applications**

**Nandkishor B. Shirsath and Tulsidas S. Savale**

*Department of Chemistry, MGVS M.S.G. Arts, Science and Commerce College, Malegaon, Savitribai Pule Pune University, Pune (MH)  
E-mail : shirsathnandkishor91@gmail.com*

A Very fine nanosized metal oxide, namely, iron oxide has been synthesized by precipitation method using ammonia as precipitating agent and characterized by using XRD (X-ray diffraction), TGA/DTA, surface area measurement (FE-SEM), and magnetic measurements techniques. Magnetic measurements showed that iron oxide has five unpaired electrons and is ferromagnetic in nature,  $M_s$  value being 1.7 emu/g. The particle size of the synthesized iron oxide was determined by FE-SEM. Over the years, many different iron oxide nanoparticles have been evaluated for a wide range of biomedical applications. The synthesized magnetic iron oxide nanoparticles have applications in pharmaceutical science, specifically for cell labelling, tissue repair, cancer treatment, immunotherapy, and stem cell therapy. More research in biomedicine should be conducted using different methods.

### **IP-CYSA-02: Improved Electrochemical Detection of 2,4,6-trichlorophenol using Cu-doped Biocarbon Derived from Green Pea Peels**

**Shambhavi G. Salimath<sup>1</sup>, Ranjan S. Shetti<sup>2</sup> and Nagaraj P. Shetti<sup>2\*</sup>**

*<sup>1</sup>Department of Mechanical Engineering, K.L.E. Institute of Technology, Hubballi -580027, Karnataka*

*<sup>2</sup>Center for Energy and Environment, School of Advanced Sciences, KLE Technological University, Hubballi - 580031, Karnataka  
E-mail : npshetti@kletech.ac.in; salimath576@gmail.com*

Copper-doped activated carbon derived from green pea peels

(GPPB) was deployed as a modifier for a CTAB-assisted carbon paste electrode (CTAB-GPPB/CPE) to enable sensitive detection of 2,4,6-trichlorophenol (2,4,6-TCP). Comprehensive physicochemical characterization confirmed the purity, structure, morphology, crystallinity, elemental composition, and distribution of GPPB, while the modified electrode exhibited superior conductivity and enlarged surface area. Electrochemical measurements revealed a significantly smaller semicircle in the impedance spectra for GPPB/CPE compared to the bare electrode, indicating substantially lower charge-transfer resistance and faster interfacial electron transfer at the modified surface. At pH 6.0, the sensor achieved a detection limit of 1.24 nM and a quantification limit of 3.78 nM, with two linear ranges (1.2–8.0  $\mu$ M and 8.0–18.0  $\mu$ M), reflecting an excellent dynamic range and high sensitivity. The sensor demonstrated robust selectivity against common interferents and satisfactory recoveries in spiked environmental samples, underscoring its practical applicability for environmental monitoring. Overall, the results validate GPPB as a functional carbon material for scalable, green chemistry-driven sensing platforms and highlight the advantageous role of surface modification in enhancing electrochemical performance for the detection of trace 2,4,6-TCP.

### **IP-CYSA-03: Development of MOF-5@CMTS Nano Heterojunction-based PVDF Polymer Composites for UV Shielding Applications**

**Veda B.P., Chandana N., Bharath Kumar S.P., Kumaraswamy N.\***

*Department of Chemistry, Sri Jayachamarajendra College of Engineering, JSS Science and Technology University, Mysuru - 570006, Karnataka  
E-mail : kumaryagati@gmail.com; vedaprabhuswamy@jssstuniv.in*

MOF-5@CMTS nanoparticles were synthesized via a hydrothermal method, and PVDF/MOF-5@CMTS nanocomposites were created using a solution-casting technique with different filler concentrations (0.0, 1.0, 3.0, and 5.0 wt%). Structural and morphological analyses were performed with X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), Raman spectroscopy, scanning electron microscopy (SEM), and high-resolution transmission electron microscopy (HR-TEM), confirming the successful integration of MOF-5@CMTS nanoparticles into the PVA matrix, along with even dispersion and strong interfacial bonding. Optical analyses using UV–Visible spectroscopy showed increased absorption in the UV range (200–370 nm), along with a systematic decrease in the optical band gap as the MOF-5@CMTS content increased. The direct band gap lowered from 4.81 to 2.80 eV, and the indirect band gap decreased from 2.81 to 2.71 eV, indicating

the nanocomposites behave as direct semiconductors. A drop in Urbach energy to 0.78 eV signified improved structural order and fewer defects. Key optical constants, including refractive index, extinction coefficient, optical conductivity, and dispersion parameters, were calculated, along with the zero-frequency dielectric constant. Photoluminescence spectra displayed emission shifts with a large Stokes shift (~180 nm), confirming efficient photon down-conversion. Dielectric relaxation and AC electrical properties measured from 20 Hz to 10 MHz revealed an 80% boost in dielectric performance, and electrical conductivity increased with higher MOF-5@CMTS loadings. Overall, the notable enhancement in optical absorption, dielectric behavior, and electrical conduction demonstrates that PVDF/MOF-5@CMTS nanocomposites are suitable for tunable UV-shielding, exhibiting excellent linear and nonlinear optical properties and strong luminescence, making them promising for advanced UV-protective coatings, optoelectronic devices, and nonlinear photonic systems.

### **IP-CYSA-04: Fabrication of MOF-5/rGO@SrCuO<sub>2</sub> Nanocomposite-based PVDF Polymer Composite Films for Photonic Application**

**Indushree Veerananje<sup>1</sup>, Chandana N.<sup>1</sup>,  
Veda Bandigowdanahalli Prabhuswamy<sup>1</sup>,  
Sanjay Ballur Prasanna<sup>2</sup> and Kumara Swamy Ningappa<sup>1\*</sup>**

<sup>1</sup>*Department of Chemistry, Sri Jayachamarajendra College of Engineering, JSS Science and Technology University, Mysuru - 570006, Karnataka*

<sup>2</sup>*Department of Chemical Engineering and Biotechnology, National Taipei University of Technology (Taipei Tech), Taipei 10608, Taiwan*  
E-mail : kumaryagati@gmail.com; chandananaik@jssstuniv.in

Herein, the MOF-5/rGO@SrCuO<sub>2</sub> hybrid nanocomposite with a well-defined heterojunction structure was successfully synthesized using the sonication method. The study focuses on incorporating these nanocomposites into a polyvinylidene fluoride (PVDF) matrix at different weight percentages (0, 0.5, 1.5, 3 and 5 wt%) to create PVDF/MOF-5/rGO@SrCuO<sub>2</sub> polymer nanocomposites. Various characterization techniques were employed to examine how MOF-5/rGO@SrCuO<sub>2</sub> influences the PVDF polymer matrix and its structure, morphology as well as optoelectronic properties. These techniques included X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), Energy Dispersive X-ray Spectroscopy (EDS), Scanning Electron Microscopy (SEM), High-Resolution Transmission Electron Microscopy (HR-TEM), Photoluminescence (PL), UV-Visible spectroscopy, and water contact angle analysis. As filler content increased, the produced



nanocomposites showed significant improvements in crystallinity, interfacial compatibility, and overall optical performance. The UV-blocking performance of the 5 wt% PVDF/MOF-5/rGO@SrCuO<sub>2</sub> composition was excellent, exhibiting strong absorption in the 245-380 nm range, a reduced optical bandgap, and lower Urbach energy. This formulation also demonstrated a distinct shift in surface properties from hydrophilic to hydrophobic, along with an increase in luminescence intensity. Furthermore, considerable enhancements were observed in both linear and nonlinear optical susceptibility measures, indicating high optical responsiveness. Overall, these findings demonstrate the nanocomposite's exceptional structural integrity and multifunctional optical capabilities, emphasizing its potential for use in optoelectronic devices and effective UV-shielding applications.

### **IP-CYSA-05: Development of Highly Efficient MIL-53(Fe)@SrCuO<sub>2</sub>@RGO Electrocatalyst for the Alkaline Water Splitting Applications**

**Rakshith G.N.<sup>1</sup>, Bharath Kumar S.P.<sup>1</sup>, Sunith Kumar K.A.<sup>1</sup>, Chetana S.<sup>2\*</sup> and Kumara Swamy N.<sup>1\*\*</sup>**

<sup>1</sup>*Department of Chemistry, JSS Science and Technology University, Mysuru-570006*

<sup>2</sup>*Department of Mechanical Engineering, ATME College of Engineering, Mysore-570028*

*E-mail: kumaryagati@gmail.com; chetana.s.mech@gmail.com; rakshithgn642004@gmail.com*

Herein, the development of highly efficient and cost effective electrocatalyst viz MIL-53(Fe)@SrCuO<sub>2</sub>@RGO, was investigated for the alkaline water splitting applications. MIL-53(Fe)@SrCuO<sub>2</sub>@RGO nanoheterojunction catalyst was prepared by hydrothermal method and the physical characterization was performed using XRD, FTIR, HR-TEM, XPS, and Raman spectroscopy to elucidate its crystal structure, chemical bonding, morphology, and surface composition. Further, the heterostructure was used to fabricate Nickel foam electrode (Ni/MIL-53(Fe)@SrCuO<sub>2</sub>@RGO) and its electrocatalytic activity towards Oxygen evolution reaction (OER) and Hydrogen evolution reaction (HER) was evaluated in alkaline medium through cyclic voltammetry (CV) and linear sweep voltammetry (LSV). The electrochemical performance evaluated through CV, LSV, electrochemical impedance spectroscopy (EIS), and Tafel analysis revealed a low overpotential of 184.69 mV for OER activity at a current density of 10 mA/ cm<sup>-2</sup>, demonstrating superior intrinsic activity and rapid kinetics. The optimum overpotential for the HER activity was found to be 636 mV at a current density of 10 mA. The OER and HER activities of the proposed Ni/MIL-53(Fe)@SrCuO<sub>2</sub>@RGO electrode were found to be excellent compared to many electrode materials reported in literature. The findings from the study suggest that the designed



nanomaterial act as a robust electrocatalyst for the water splitting process and has the potential to be used in energy conversion applications.

## **IP-CYSA-06: Bio-Waste Derived Nitrogen-Doped Activated Carbon for the Electrochemical Sensing of Bisphenol A**

**Sharadeeshri H.K.<sup>1</sup>, Madasu Sreenivasulu<sup>2</sup> and Nagaraj P. Shetti<sup>2\*</sup>**

<sup>1</sup>*Department of Mechanical Engineering, K.L.E. Institute of Technology, Hubballi -580027, Karnataka*

<sup>2</sup>*Center for Energy and Environment, School of Advanced Sciences, KLE Technological University, Hubballi - 580031, Karnataka*  
*E-mail: npshetti@kletech.ac.in*

Bisphenol A (BPA) is an endocrine-disrupting compound widely present in plastic packaging, necessitating the need for reliable environmental monitoring. This work reports a bio-derived electrochemical sensor based on nitrogen-doped sweet potato peel-derived activated carbon (NSC), synthesised from sweet potato biowaste, enabling sensitive detection of BPA. The NSC materials were prepared via a single-step pyrolysis-activation process at 400–600 °C, yielding NSC-400 to NSC-600, and were comprehensively characterised by various analytical techniques, confirming a highly porous, nitrogen-enriched carbon framework with enhanced surface functionality. The NSC-600 / carbon paste electrode exhibited an electrochemically active surface area of 0.051 cm<sup>2</sup>, attributed to hierarchical porosity and improved charge-transfer pathways. BPA detection proceeded through a diffusion-controlled oxidation process involving equal numbers of protons and electrons, as evidenced by cyclic voltammetry and electrochemical impedance spectroscopy. A low detection limit of 9.2 nM (S/N = 3) and two linear ranges (1.2–8.0 µM and 8.0–18.0 µM) demonstrated a wide dynamic range and high sensitivity. The sensor demonstrated good selectivity against common interferents, excellent reproducibility, and stable performance over a 30-day period. Real-sample testing in spiked water and soil extracts yielded recoveries ranging from 96% to 103%, confirming the practical applicability of the method.

## ORGANIC CHEMISTRY SECTION

### Sectional President's Address

#### **Organic Chemistry-Inspired Zwitterionic Polymers for Advanced Membrane Performance**

**Arun M. Isloor**

*Membrane and Separation Technology Laboratory, Department of Chemistry,  
National Institute of Technology Karnataka, Surathkal, Mangalore-575 025  
E-mail : isloor@yahoo.com*

Zwitterionic molecules, from an organic chemistry perspective, are fascinating structures that contain intrinsic charge separation—a positively charged functional group and a negatively charged functional group within the same molecule. This internal balance of charges allows them to engage in strong, highly ordered hydrogen-bonding interactions with surrounding water molecules. As a result, zwitterions generate a robust hydration shell that minimizes nonspecific interactions by preventing external molecules from adhering to zwitterionic surfaces.

When such zwitterionic moieties are integrated into nanoparticles, this hydration layer becomes especially valuable. It protects the particle surface from protein adsorption and immune recognition, thereby prolonging circulation time and improving the efficiency of drug delivery systems. The same organic-chemical principles—charge distribution, hydrogen-bonding capacity, and hydrophilic functional group behavior—have inspired the incorporation of zwitterionic units into polymeric membrane matrices. These modifications enhance membrane hydrophilicity, permeability, and most importantly, antifouling performance, an outcome tied directly to the molecular-level interactions of zwitterionic groups with water and solutes.

Despite significant progress, substantial scope remains for experimental exploration, particularly in evaluating how zwitterion-modified membranes perform against complex contaminants such as natural organic matter, dyes, heavy-metal ions, pesticides, and pharmaceutical residues.

## **IOL-01 : Understanding the Morphology Depended Photophysical Behaviour in Donor- Acceptor Systems**

**Vandana Bhalla\***

*Department of Chemistry, UGC Sponsored-Centre of Advance Studies-II, Guru Nanak Dev University, Amritsar, Punjab-143005  
E-mail: vanmanan@yahoo.co.in*

Our research work aims at development of donor-acceptor building blocks which undergo self-assembly in aqueous media to generate fluorescent assemblies in aqueous media.<sup>1-5</sup> These assemblies having appropriate binding sites for interactions with specific analytes undergo guest induced morphology transformation and exhibit interesting photophysical properties. Very recently, we have developed supramolecular assemblies having chiral -handle and investigated the achiral/chiral guest induced chirality transformations in aqueous media.<sup>4-5</sup> Furthermore, we have also developed metal based as well as metal free supramolecular catalytic ensembles for carrying out various organic transformations. In the presentation, different aspects of development of these 'lighted' materials and their molecular recognition and catalytic applications will be discussed.

## **IOL-02 : Fluorescence Modulation in an ESIPT-Active Columnar Liquid Crystal via Quantum Dot Interaction**

**C. V. Yelamaggad<sup>1,2\*</sup>**

*Centre for Nano and Soft Matter Sciences (CeNS)*

<sup>1</sup>*Arkavathi, Survey No.7, Shivanapura, Dasanapura Hobli, Bengaluru-562162*

<sup>2</sup>*SJB Institute of Technology, Health & Education City, Kengeri, Bengaluru - 560060*

*E-mail: yelamaggad@cens.res.in/ yelamaggad@gmail.com*

The modulation of luminescent behavior of organic fluorophores has remained a key objective in contemporary research. Various strategies have been adopted to overcome inherent limitations, including short absorption and emission wavelengths, small Stokes shifts, low quantum efficiency, limited permeability, poor photostability, and low solubility. The approaches based on binary or multicomponent systems integrating organic and inorganic functional materials have emerged as particularly promising and enduring. Working in this direction, elaborative studies have been carried out on the photoluminescence of organic and hybrid composites formed by incorporating (doping) organic dyes and quantum dots (QDs) into an ESIPT-active columnar (Col) liquid crystal (LC) host. The binary mixtures have been prepared by doping organic dyes such as methyl red/rubrene and carbon QDs/perovskite (CsPbBr<sub>3</sub>) QDs in a fluorescent

(ESIPT) Col LC, namely, phasmidic bis(N-salicylideneaniline) (abbreviated as PBSAN-14). The photophysical investigations have been carried out in their solutions and three condensed states, viz., solid, LC, and liquid states. The organic dye–Col LC composites suppress photoluminescence, as indicated by Stern–Volmer analysis, revealing both dynamic and static quenching mechanisms. The Col LC–QD composites emit light intensively, spanning nearly the entire visible regime. This study provides invaluable insights into the influence of organic dyes and quantum dots on the photophysical behavior of fluorophores in the condensed state.

### **IOL-03 : Fluorescence Modulation in an ESIPT-Active Columnar Liquid Crystal via Quantum Dot Interaction**

**C.V. Yelamaggad<sup>1,2\*</sup>**

*Centre for Nano and Soft Matter Sciences (CeNS)*

<sup>1</sup>Arkavathi, Survey No.7, Shivanapura, Dasanapura Hobli, Bengaluru-562162

<sup>2</sup>SJB Institute of Technology, Health & Education City, Kengeri, Bengaluru – 560060

E-mail: yelamaggad@cens.res.in; yelamaggad@gmail.com

The modulation of luminescent behavior of organic fluorophores has remained a key objective in contemporary research. Various strategies have been adopted to overcome inherent limitations, including short absorption and emission wavelengths, small Stokes shifts, low quantum efficiency, limited permeability, poor photostability, and low solubility. The approaches based on binary or multicomponent systems integrating organic and inorganic functional materials have emerged as particularly promising and enduring. Working in this direction, elaborative studies have been carried out on the photoluminescence of organic and hybrid composites formed by incorporating (doping) organic dyes and quantum dots (QDs) into an ESIPT-active columnar (Col) liquid crystal (LC) host. The binary mixtures have been prepared by doping organic dyes such as methyl red/rubrene and carbon QDs/perovskite (CsPbBr<sub>3</sub>) QDs in a fluorescent (ESIPT) Col LC, namely, phasmidic bis(N-salicylideneaniline) (abbreviated as PBSAN-14). The photophysical investigations have been carried out in their solutions and three condensed states, viz., solid, LC, and liquid states. The organic dye–Col LC composites suppress photoluminescence, as indicated by Stern–Volmer analysis, revealing both dynamic and static quenching mechanisms. The Col LC–QD composites emit light intensively, spanning nearly the entire visible regime. This study provides invaluable insights into the influence of organic dyes and quantum dots on the photophysical behavior of fluorophores in the condensed state.

## **IOL-04 : Discotic Liquid Crystals: Next Generation Materials for Organic Electronics**

**A. S. Achalkumar**

*Department of Chemistry, Indian Institute of Technology Guwahati,  
Guwahati, 781039, Assam*

*\*E-mail: achalkumar@iitg.ac.in*

Liquid crystalline semiconductors seem to be a bright option for the application in organic electronics considering their good solubility, processability and excellent reproducibility along with the ease of purification. Additionally, the addressability of their molecular alignment and self-healing of defects in the thin films by thermal annealing provides a major advantage over amorphous polymers and organic single crystals. This presentation reports several shape anisotropic molecules that stabilize columnar (Col) phases. Col phases are formed by the one-dimensional stacking of the disk/star/polycatenar shaped molecules, leading to an intimate overlap of the central aromatic units. The molecular design of these molecules is such that, they are able to form spontaneous columnar organization in response to stimuli like solvent and/or temperature. The Col phase provides a one-dimensional (1D) pathway for the migration of charge carriers akin to ‘molecular wires’. Our present focus is on the application of such Col LCs in enhancing the efficiency in organic electronic devices such as organic solar cells (OSCs), organic light emitting diodes (OLEDs) and organic field effect transistors (OFETs). As expected, the gaps between the expectation and the performance of the molecules in such devices are to be addressed, which we are working on through the experience. In this presentation, I will be discussing our recent research on various polyaromatic molecules stabilizing columnar mesophases.<sup>6-7</sup>

## **IOL-05 : Current Trends in Organic Synthesis for Sustainable Process Developments in the Pharmaceutical Industry**

**Vijayavithal T. Mathad**

*CRAMSN Research Park (P) Ltd., MSN Group of companies, Hyderabad*

The Indian pharmaceutical industry, widely recognized as the “Pharmacy of the World,” is undergoing a critical paradigm shift from traditional volume-based manufacturing to sustainable and value-driven process development. As global environmental regulations tighten and the demand for green supply chains increases, Indian manufacturers are increasingly adopting Green Chemistry principles to maintain cost-competitiveness and ecological compliance.

The current trends in organic synthesis within the Indian sector, specifically focusing on the transition from batch to continuous flow chemistry, the integration of bio-catalysis (enzymatic reactions), and the use of eco-friendly solvents. Furthermore, it analyses the impact of these innovations on reducing the E-factor (waste-to-product ratio) and improving atom economy in Active Pharmaceutical Ingredient (API) production. This concludes that sustainable process development is no longer just a regulatory requirement but a strategic asset for the Indian pharmaceutical industry to secure its future in the global market.

Thus, this talk mainly focussed on discussing the challenges and opportunities associated with “Green chemistry” in Pharmaceutical Development and Manufacturing with few case studies.

### **IOL-06 : Dipolar Addition Reaction – A Facile Route in the Synthesis of Novel Bio-Active Molecules**

**Balakrishna Kalluraya**

*Department of Chemistry, Mangalore University, Mangalagangothri-574199  
E-mail : bkalluraya@gmail.com*

In this presentation a brief review on the application of dipolar addition approach for the synthesis of bioactive molecules used in pharmaceutical industry and its advantages and the modern trends in drug design will be discussed.

### **IOL-07 : Greener Syntheses Employing Heteroallenes: An Easy Access for the Syntheses of Biologically Potent Scaffolds**

**Devdutt Chaturvedi\***

*Department of Chemistry, School of Physical Sciences, Mahatma Gandhi Central University, Motihari-845401(East Champaran), Bihar  
E-mail : devduttchaturvedi@gmail.com; devduttchaturvedi@mgcub.ac.in*

In recent years, development of novel synthetic methodologies have been attracted a great deal of attention for organic chemists around the globe, for the synthesis of structurally diverse biologically potent molecules. The advantages associated with these synthetic methodologies are lesser synthetic steps, use of cheaper and safer new alternatives, involves overall lesser reaction time, milder reaction conditions, and afforded high yields. Extensive efforts have been made by organic chemists around the globe and thus developed several kinds of new and highly efficient methods for the generation of various kinds of structurally diverse molecules of biological significance.

In recent years, carbon dioxide/carbon disulfide/carbonyl sulfide has been employed as a cheap and safe alternative eliminating the use of harmful reagents such as CO and COCl<sub>2</sub>. Recently, carbon dioxide/carbon disulfide/carbonyl sulfide has frequently been employed as a green reagent in its various conditions and forms for the syntheses of structurally diverse biologically potent scaffolds employing diversity of starting materials, reagents and catalytic systems. In the present talk, we will focus some of our novel and efficient methods for the synthesis of biologically potent scaffolds.

## **IOL-08 : Sustainable Organic Synthesis Using Green Technology for Chemical Industries**

**K.R. Desai**

*Ukatarsadia University*

*Bardoli-Mahuwa-Road, Surat-(Gujarat)*

Sustainability is the index of development of the modern society and in the context of chemistry it can be achieved adopting the green chemistry principles. This has urged the industry and academia to aim sustainable development of chemistry. The demands for green and sustainable synthetic methods in the fields of pharmaceutical industries, healthcare and fine chemicals combined with the pressure to produce these substances expeditiously and in an environmentally benign fashion, pose significant challenges to the synthetic chemical community. Green chemistry protects the environment, not by cleaning it up but by inventing new chemistry and new chemical processes that do not pollute.

In my talk I will mainly focus on Green Brominating technique, Green Diazotization technique, Green Reduction, Oxidation and many others Green methods. This may be by changing catalyst, solvent or source of energy, Biocatalyst etc.

Moreover, to overcome the difficulties arising from conventional methods, there is continuous growing research interest to improve the reactions either in basic research or in technology in context to green chemistry. Also focus on increasing selectivity, aiming for 100% atom efficiency and replacing Stoichiometric reagents, with heterogeneous reusable catalyst. The nano-sized particles increase the exposed surface area of the active component of the catalyst, thereby enhancing the contact between reactants and catalyst dramatically and mimicking the homogeneous catalysts.



## OO-01 : Design, Synthesis and Screening of Novel Triazolo-Thiazole Integrated Pyrrole Derivatives as Potent Anti-Tubercular Agents

**Pradeep Kumar M.R.**

*Department of Pharmaceutical Chemistry, KLE College of Pharmacy, HUBLI-580031, Karnataka*

*E-mail : d-pradeepmrpk@yahoo.co.in*

**Background:** Tuberculosis (TB), caused by *Mycobacterium tuberculosis*, is a chronic infectious air-borne disease. Anti-tubercular drugs (ATDs) are essential for treatment. Though the drugs are available for treating TB, due to existence of XDR and MDR-TB strains, there is an urgent need for developing potent anti-TB. In this study, the novel Pyrrole moieties were synthesized and examined as potential therapeutic drugs for the treatment of TB, which aims to address the limitations of existing anti-tubercular drugs.

**Objective:** To synthesize novel pyrrole derivatives as potent anti-TB agents.

**Methodology:** Titled compounds were synthesized by the reaction between Pyrrolyl-phenyl amino triazole thiol and substituted aromatic acids in phosphoryl chloride under controlled reflux conditions. The synthesized compounds were characterized by spectral characterization and screened In-vitro by Microplate Alamar Blue assay (MABA) method against tuberculosis H<sub>37</sub> RV strain. Compounds are further screened by in-silico method to know their binding and druggability.

**Result:** Among the series PR-1A, PR-1B, PR-1C, PR-1E, PR-1F, and PR-1L exhibited potent anti-tubercular activity.

**Conclusion:** The experimental findings indicate that the pyrrole derivatives with slight structural modification can potentially produce new effective drugs for treating tuberculosis.

## OO-02 : Chemistry of Ketone Bodies and its Impact on Human

**Amit Gupta<sup>1</sup>, Abhay Gupta<sup>2</sup>, Jaya Gupta<sup>2</sup> and Aseem Gupta<sup>3</sup>**

*<sup>1</sup>Department of Chemistry, Institute of Basic Sciences, Dr. Bhimrao Ambedkar University, Khandari Campus, Agra*

*<sup>2</sup>Department of Chemistry, Agra College, Agra*

*<sup>3</sup>S.N. Medical College Agra*

*E-mail: gamit8205@gmail.com; jayagupta6250@gmail.com;*

*aseem10850@gmail.com*

The ketone bodies i.e., acetone, acetoacetate and D-â-hydroxybutyrate are formed in the liver. The latter two compounds travel in the blood to other tissues, where they serve as fuel molecules;

they are oxidized to acetyl CoA and enter the citric acid cycle. Over production of ketone bodies in uncontrolled diabetes or severe starvation can lead to acidosis or ketosis. Diabetic keto acidosis is a serious complication of diabetes that can cause dehydration, rapid breathing, abdominal pain, in severe cases coma or death. In the present work data collected from several peoples who suffer from diabetes. On the basis of their data a conclusion is drawn that monitoring and minimizing ketones body level in the body is must in diabetic peoples.

### **OO-03 : Catalyst-Free Divergent Synthesis of 4-((2-(4-aryl)Imidazo[1,2-a]pyridin-3-yl)methyl Scaffolds with a Morpholine Moiety**

**Venkatesh K. Bhovi<sup>1\*</sup>, Sulochana P. Melinmath<sup>2</sup> and Ranjith P.B.<sup>3</sup>**

<sup>1</sup>*Department of Chemistry, Vijayanagar College, Hosapete Vijayanagar, Karnataka-583201.*

<sup>2</sup>*Department of chemistry Kishkinda University, BITM campus Ballari, Ballari 583104, Karnataka*

<sup>3</sup>*Department of Chemistry, Karnataka University Dharwad, Dharwad-580003*

A novel, catalyst-free synthetic strategy has been adopted for the synthesis of a diverse library of functionalized 2 functionalized 2-phenylimidazo[1,2-a]pyridine and 4-((2-phenylimidazo[1,2-a]pyridin-3-yl)methyl)morpholine(4a-o) derivatives. This environmentally benign approach proceeds via a one-pot condensation of various substituted 2-aminopyridines and  $\alpha$ -bromo ketones (substituted phenyl bromide), followed by a Mannich-type cyclization with morpholine to afford the title compounds in good yields under mild conditions. These compounds were confirmed by analytical techniques, such as, IR NMR and Mass spectroscopy. Preliminary biological evaluation revealed that several of these novel molecular hybrids exhibit notable antimicrobial efficacy, outperforming a standard drug in initial assays. A clear structure-activity relationship was observed, indicating that the nature of the aromatic substituent plays a critical role in modulating the biological activity, with specific functional groups conferring enhanced potency.

### **OO-04 : Artificial Intelligence in Drug Discovery and Development**

**Dinesh Kanade<sup>1</sup> and V.S. Shrivastava<sup>2</sup>**

<sup>1</sup>*Assistant Professor & Head, Department of Chemistry, Govt. P. G. College Sendhwa, Dist.-Barwani (MP)*

<sup>2</sup>*Former Principal and Director, GTP College Nandurbar, Maharashtra-425412  
E-mail: prof.dinesh.kanade@gmail.com*

The integration of Artificial Intelligence (AI) in medicinal chemistry has transformed the drug discovery and development landscape. AI's

ability to analyze vast amounts of data, identify complex patterns, and make accurate predictions has accelerated the identification of potential drug candidates, optimized lead compounds, and predicted their efficacy and toxicity. This abstract highlights the applications of AI in medicinal chemistry, including virtual screening, de novo drug design, and predictive modeling of pharmacokinetic and pharmacodynamic properties. AI-driven approaches have shown promise in identifying novel targets, designing molecules with desired properties, and predicting off-target effects.

#### Applications and Benefits:

AI has been successfully applied in various areas of medicinal chemistry, including:

**Drug discovery:** AI to optimize the design of drug molecules, chemists can create new drugs that are more effective and have fewer side effects.

**Materials Science:** Deep learning models can be used to predict the melting point of a new material based on its crystal structure. These models can also identify new materials with desirable properties, such as high thermal conductivity or low toxicity.

**Virtual screening:** AI algorithms can rapidly screen large libraries of compounds to identify potential hits.

**De novo drug design:** AI can design novel molecules with desired properties.

**Predictive modeling:** AI can predict pharmacokinetic and pharmacodynamic properties, reducing the need for experimental testing.

## **OO-05 : Computational Screening of Alpha-Glucosidase Inhibitors from Lactuca Serriola Linn**

**Kailash S. Chadchan<sup>1</sup>, Swastika N. Das<sup>1</sup> and Prachi Parvatikar<sup>2</sup>**

<sup>1</sup>*Department of Chemistry, BLDEA's V.P. Dr. P.G. Halakatti College of Engineering and Technology, Vijayapura, Karnataka*

<sup>2</sup>*Department of Biotechnology, School of Applied Science and Technology, BLDE(DU), Vijayapura, Karnataka*

Alpha-glucosidase inhibitors play a crucial role in managing postprandial hyperglycemia in type 2 diabetes mellitus by delaying carbohydrate digestion and absorption. In the present study, an in silico approach was employed to evaluate the alpha-glucosidase inhibitory potential of phytocomponents present in Lactuca serriola Linn, a green leafy vegetable often consumed as a salad by the people of north Karnataka region. A comprehensive literature survey was

conducted to identify and compile the major phytochemical constituents of the plant. Molecular docking studies were then performed using Flare Pro Plus software to assess the binding affinity of each phytocomponent against the alpha-glucosidase enzyme. Among the screened compounds, Luteolin exhibited the most promising interaction with a significant docking score of -7.028 kcal/mol, suggesting strong inhibitory potential. The docking interactions revealed favourable binding conformations and key hydrogen bonding interactions within the enzyme's active site. These findings indicate that Luteolin, a naturally occurring flavonoid in *Lactuca serriola* Linn, may serve as a lead compound for the development of novel alpha-glucosidase inhibitors. Further in vitro and in vivo studies are to be performed to validate these computational predictions.

### **OO-06 : Direct N-H/N-Me Aziridination of En ones**

**Ajay K. Yadav<sup>1</sup>, Abhay Krishna<sup>2</sup> and Jawahar L. Jat<sup>3</sup>**

<sup>1</sup> Department of Chemistry, K. M. C. Language University,,Lucknow-226013, UP

<sup>2</sup> Dept. of Applied Sciences & Humanities, K. M. C. Language University

Lucknow, UP, India-226013,,<sup>3</sup> Department of Chemistry, School of Physical & Decision Sciences,,Babasaheb Bhimrao Ambedkar University (A Central University), Lucknow-226025 (U.P.)

E-mail : ajayy473@gmail.com

N-H/N-Me aziridine moiety present in various bio-active natural, synthetic and semi-synthetic molecules. They also serve as a versatile building blocks in organic synthesis and they can undergo various transformation reactions such as ring opening, ring expansion and rearrangements. The syntheses of activated aziridines from olefins are well established while the direct methods for non-activated aziridines from enones are less explored. Herein we describe the highly efficient direct method for the synthesis (N-H/N-Me) aziridines from enones using O-(sulfonyl) hydroxylamine as the aminating agent.

### **OO-07 : Highly Efficient Green Synthesis of Novel tetrahydrobenzo[b]thiophene-3-carboxylate Derivatives via Cu-Catalyzed Click Chemistry in Ionic Liquids: A Novel Sonochemical Approach of synthesis, Biological Evaluation, and Computational Insights**

**Sunita Kurahattia and Rajesh G. Kalkhambkara\***

Department of Chemistry, Karnatak University's Karnatak Science College, Dharwad, Karnataka 580001

E-mail: kurahattisunita@gmail.com

A series of novel tetrahydrobenzo[b]thiophene-3-carboxylate derivatives were synthesized efficiently via copper catalysed azide-

alkyne cycloaddition in an ionic liquid medium under ultrasonication at 50/ °C in 3/ h. The methodology combines mild reaction conditions with excellent atom economy and low waste generation. The green solvent ionic liquid could be recycled over multiple cycles (up to 7) without significant loss of efficiency, demonstrating its potential as a green and sustainable reaction medium. To complement the experimental findings, density functional theory (DFT) calculations were performed to probe the electronic properties, while molecular docking studies provided insights into the binding interactions with relevant biological targets. Collectively, this study demonstrates a practical, sustainable, and versatile approach for accessing tetrahydrobenzo[b]thiophene-3-carboxylate based scaffolds with potential biomedical applications.

### **OO-08 : Copper Nanoparticles Synthesized from Commelina forskalaei as Natural Antimicrobials: A Green Approach Against Pathogenic Microbes**

**S. P. Vyas**

*Department of Chemistry,, The HNSB. Ltd. Science College, Himatnagar-383001  
E-mail: vyasspraghav0763@gmail.com*

This study presents the green synthesis of copper nanoparticles (CuNPs) using aqueous extracts of *Commelina forskalaei*, offering a sustainable and eco-friendly alternative to conventional chemical synthesis methods. The biosynthesized CuNPs were thoroughly characterized using UV–Vis spectroscopy, FTIR, SEM, EDS, TEM, and XRD analyses. Phytochemical screening of the plant extract confirmed the presence of alkaloids, flavonoids, phenols, and other secondary metabolites, which acted as natural reducing and stabilizing agents during nanoparticle formation.

The biological activities of the synthesized CuNPs were assessed through antioxidant and antimicrobial assays. The DPPH assay demonstrated notable free radical scavenging activity, indicating strong antioxidant potential. Furthermore, the CuNPs exhibited significant antibacterial and antifungal effects, with the highest inhibition zones observed against selected pathogenic microbes.

These findings reveal that plant-mediated synthesis of CuNPs not only provides a green and sustainable route for nanoparticle production but also yields materials with promising therapeutic and biomedical potential. The study underscores the importance of eco-friendly nanotechnology for developing functional materials that combine high biocompatibility with minimal environmental impact.

## **OO-09 : Harnessing Natural Chromenes for the Development of Novel Estrogen Receptor Ligands through Structural Refinements**

**Atul Gupta**

*Phytochemistry Division, CSIR-Central Institute of Medicinal and Aromatic Plants, P.O. CIMAP, Kukrail Road, Lucknow-226015  
E-mail : a.gupta@cimap.res.in*

Receptors are proteinous macromolecules in apo form under normal/ unliganded conditions. As the ligand approaches a receptor, it brings specific molecular changes; ultimately resulting in the receptor's stereo-chemical changes, especially in the ligand binding pocket of the receptor.<sup>1</sup> The stereochemistry of the ligand molecules mainly dictates these changes. Often, the molecular flexibility of a ligand offers effective electrostatic interactions between amino acid residues of the ligand-binding protein (LBP) of the receptor and ligand.<sup>2</sup> These observations indicated that interplay with the stereochemistry of triaryl-ethylene cores, as present in Tamoxifen, and relocation of the alkyl amine side chain improve biological activity through the enhanced affinity of ligands with target proteins via efficient interactions. It is also assumed that such molecules may elicit better pharmacological activity than their stereochemical rigid counterparts. Accordingly, substituted dimethyl-chroman-based stereo-chemically flexible and constrained Tamoxifen analogs were synthesized as anti-breast cancer agents through structural modifications of natural chromene isolated from *Ageratum conyzoides* (L.) L.<sup>3,4</sup> The synthesized compounds showed significant anti-proliferative activity against estrogen receptor-positive (ER+, MCF-7) and negative (ER-, MDA-MB-231) cells within an IC<sub>50</sub> value of 8.5-25.0  $\mu$ M. Amongst all, four potential molecules were evaluated for their effect on the cell division cycle and apoptosis of ER+ and ER- cancer cells (MCF-7 & MDA-MB-231cells), which showed that these compounds possessed anti-proliferative activity through triggering apoptosis. In-silico docking experiments elucidated the possible affinity of compounds with estrogen receptors- $\alpha$  and - $\beta$ .

## **OO-10 : Synthetic Utility of 1-hydroxyimino-2,3,4,9-tetrahydro-carbazoles- An Attempted Synthesis of Aminocarbazoles**

**Sridharan M.A.**

*Department of Chemistry, R.V. College of Engineering, Bangalore-560059, Karnataka  
E-mail : sridharanm@rvce.edu.in*

An attempted synthesis of 1-aminocarbazoles (2) from 1-

hydroxyimino-2,3,4,9-tetrahydrocarbazoles (1) resulted in the formation of new heterocyclic ring fused carbazoles. The spectral and analytical data showed the possibility for two structures, imidazo [4,5,1-j,k] carbazol-3-ol (4) or oxazolo[4,5-a]carbazole (5). Final conclusive proof for the formation of 4 over 5 was rendered by acetylating the product using acetic anhydride and pyridine to yield O-acetylated compound rather than N-acetylated compound. A plausible mechanism for the formation 5 from 1 has been proposed (Scheme 1) . Thus we have been able to develop a new short approach towards the imidazo carbazoles and have, as well achieved the first synthesis of this type of ring system.

## **OO-11 : Exploring Schiff Bases and Azetidinone Derivatives as Emerging Scaffolds in Antimicrobial Drug Discovery**

**Channamma M.**

*Rajiv Memorial Education Society's College of Pharmacy, Kalburagi-585102, Karnataka*

*E-mail : channagmaj@gmail.com*

The increasing prevalence of microbial resistance has limited the effectiveness of existing antibiotics, emphasizing the need for novel therapeutic agents. In this study, a series of innovative Schiff bases and their corresponding Azetidinone derivatives were synthesized to explore their antimicrobial potential.

Condensation of substituted aromatic aldehydes with free amino group of aromatic compound yielded Schiff bases which upon cyclization with Phenyl and phenoxy / acetyl chloride afforded the corresponding azetidinone derivatives (CH-01-01 to CH-01-06 & CH-02-01 to CH-02-06). The purity of synthesized compounds was confirmed by thin layer chromatography (R<sub>f</sub> values) and melting point determination. Structural elucidation of synthesized compounds (CH-01-01 to CH-01-06 & CH-02-01 to CH-02-06) was achieved through by spectral analysis (<sup>1</sup>H-NMR, <sup>13</sup>C-NMR, IR, Mass and Elemental Analysis).

Antibacterial and antifungal activities were evaluated by the Agar well diffusion method against E.Coli, S.infantis, A.niger, S.aureus, C.albicans and C.glabrata by employing Erythromycin & Ketoconazole as standards. Several Azetidinone derivatives exhibited significant antimicrobial activity, particularly those bearing electron-withdrawing substituents which enhanced lipophilicity and cell membrane penetration.

Structure-activity relationship analysis revealed that the azetidinone moiety contributed to improved biological response



indicating their potential as lead molecules for the development of new antimicrobial agents.

## **OO-12 : Synthesis of Polyhydroquinoline Using Sulfanilic Acid as a Catalyst**

**Pramod Kulkarni**

*Department of Chemistry and Post-Graduate Research Center in Organic Chemistry, Hutatma Rajguru Mahavidyalaya, Rajguru Mahavidyalaya, Rajgurunagar, Pune-410505  
E-mail : pramodskulkarni3@gmail.com*

Polyhydroquinolines (PHQs) are an important class of bioactive heterocyclic compounds exhibiting diverse pharmacological activities such as vasodilator, antihypertensive, antitumor, and neuroprotective properties. In the present study, an efficient, eco-friendly, and simple synthetic route for the preparation of polyhydroquinoline derivatives was developed using sulfanilic acid as a green catalyst. The multicomponent Hantzsch condensation of dimedone, benzaldehyde, ethyl cyanoacetate, and ammonium acetate was selected as the model reaction. Among several acids screened, sulfanilic acid was found to be the most effective catalyst, providing good yields under mild conditions. The reaction proceeds smoothly in ethanol at 70–80 °C without the need for hazardous reagents or lengthy work-up procedures. The synthesized products were characterized by IR, NMR, and mass spectroscopic analyses. This method offers several advantages such as high yield, operational simplicity, use of an inexpensive and readily available catalyst, and avoidance of toxic solvents, thereby demonstrating a sustainable and green approach for the synthesis of pharmaceutically significant polyhydroquinoline derivatives.

## **OO-13 : Synthesis of Polyvinylpyrrolidone based Polymers and their Potential use in the Tailoring of Membranes for Water Remediation**

**A.M. Vijesh**

*P.G. & Research Department of Chemistry, Payyanur College, Payyanur, Kannur University, Kerala-670327  
E-mail: vijeshnambisan82@gmail.com*

Membrane separation is an emerging technology for the fresh water reclamation either in desalination or wastewater treatment applications. Hollow fiber (HF) membranes are being used for various industrial fields such as removal of heavy metals, desalination, dye rejection, gas separation due to their selectivity, energy efficiency, ease of fabrication and environment friendly nature [1]. Polysulfone (PSf) is a commonly used membrane material due to its excellent

mechanical, chemical and thermal properties. But the hydrophobic nature of the PSf limits its use as a membrane material. In this work, properties of the PSf hollow fiber membranes were modified through one of the surface modification techniques, blending [2] with a hydrophilic polymer.

Synthesis of PVPD polymer and the fabrication of PSf-PVPD HF blend membranes: Initially polyvinylpyrrolidone hydrazone (PVPD) was synthesized from polyvinylpyrrolidone via two step reactions and confirmed by spectral studies. New PSf-PVPD HF membranes were fabricated using wet-jet phase inversion technique. The dope solution was prepared by blending PSf with polyvinylpyrrolidone-nitrobenzene (PVPD) in different compositions. 1-Methyl-2-pyrrolidone (NMP) and polyvinyl pyrrolidinone (PVP) were used as the solvent and pore forming agents respectively. The fabricated membranes were characterized by various techniques such as water contact angle, SEM, DSC, TG, IR and water uptake. Pure water flux of the membranes was measured using cross-flow filtration techniques. Dye rejection studies of the membranes were also performed and the results of such studies will be discussed in this paper.

## **OO-14 : A Convenient Synthesis of Carbamates from Halooximes and Alcohols**

**Venunath M. Hapse<sup>1,2</sup>, Pramod S. Wagh<sup>1</sup>, Ankith S.<sup>1</sup>,  
Prashantha Kamath<sup>1</sup> and Sujit K. Ghorai<sup>1,2\*</sup>**

<sup>1</sup>*Research & Technology Centre, Syngenta Biosciences Pvt. Ltd., Santa Monica Works, Corlim, Ilhas, Goa 403 110*

<sup>2</sup>*Department of Chemistry, Mangalore University, Mangalagangothri, Karnataka-576119*

Carbamates are prominent structural motifs in both pharmaceutical and agrochemical development due to their exceptional hydrogen-bonding capabilities that enable critical interactions with target proteins. These structural features enhance drug-target interactions, significantly improving biological properties including potency, selectivity, and stability. The pharmaceutical and agrochemical industries have successfully commercialized numerous products containing carbamate moieties, demonstrating their practical importance in creating effective bioactive compounds.

Synthesis of carbamates is conveniently achieved through the reaction between an isocyanate and an alcohol. Availability of commercial isocyanates is also limited, which presents a significant challenge for chemists synthesizing libraries carbamates during discovery research. This scarcity, combined with toxicity concerns of phosgene-based production methods, highlights the need for simpler

and safer synthetic alternatives having wider substrates scope. Herein, we report a metal-free, base-free, and one-pot method for preparing O-alkyl carbamates from halooxime, through the in-situ formation of isocyanates.

### **OO-15 : Phase 0 : DSST - Designing, Synthesis, Screening and Toxicity by Computational Chemistry & Green Chemistry**

**Hitesh D. Patel**

*Department of Chemistry, Gujarat University, Ahmedabad, Gujarat  
E-mail : drhiteshpatel1@gmail.com*

Drug discovery is the journey of the 10-12 years. But now the duration of the time and success rate can be improve by the computational chemistry. The synthetic organic chemist role is to design novel chemical entity by using various software and computational chemistry tools. Only the designing of the molecules is not enough for the drug discovery, but the designed organic/heterocyclic molecules should be synthesized by green chemistry approach. All synthesized compounds are purified and well characterized. The compounds are screened for the in-vitro biological activities and study the toxicity of all the highly active compounds. Since more then 15 years we are working on phase 0 (Zero). The compounds are synthesized by us are screened for anticancer, antimalarial, anti-TB, antimicrobial etc. Links or webpage for Research publicat

### **OO-16 : Development of an Analytical Method for the Enantiomeric Separation of Nine Trifluoromethylated Dihydrobenzofuran-4-ones Using Immobilized Chiral Stationary Phase**

**Gopal K. Kurhe<sup>1,2</sup>, Mahesh R. Kalbagh<sup>1</sup>, Prashantha Kamath<sup>1</sup> and Subhrakanti Saha<sup>1,2 \*</sup>**

<sup>1</sup>*Research & Technology Centre, Syngenta Biosciences Pvt. Ltd., Santa Monica Works, Corlim, IIhas, Goa-403 110*

<sup>2</sup>*Department of Chemistry, Mangalore University, Mangalagangothri, Karnataka-576119*

Trifluoromethylated dihydrobenzofuran-4-one derivatives are valuable chiral scaffolds which enhance lipophilicity, stability, and biological activity due to the presence of –CF<sub>3</sub> group. Their racemic nature implicated the need of enantiomeric separation to evaluate stereochemical behavior as well as ensure enantiopure quality for pharmaceutical and agrochemical applications. Chiral chromatographic methods are essential for these compounds to separate and quantify enantiomers. Individual chiral method development using trial and

error method is quite costly, tedious and labourious job. Here, we report a single method for enantiomeric separation of nine trifluoromethylated dihydrobenzofuran-4-one derivatives using normal phase HPLC with immobilized polysaccharide-based chiral stationary phase. The work involves a detailed column and solvent screenings followed by method development and optimization. We found that under specific chromatographic conditions Chiralpak-IB column provides the best separation for all the nine compounds. The figures of merit of the method were determined in optimized condition and were found suitable for using the enantiomeric separation of similar type of racemic compounds with baseline separation. The present work minimizes the method development time while ensuring high resolution and reproducibility, establishing a robust analytical technology for enantiomeric purity assessment of fused dihydrobenzofuranones derivatives in pharmaceutical and agrochemical ingredients.

## **OO-17 : A Versatile Synthetic Approach to Brominated Enaminone-Coumarin Hybrids with Potential Biological Relevance**

**Hari Babu Bollikolla<sup>1\*</sup> and Ravi Varala<sup>2</sup>**

<sup>1</sup>*Department of Chemistry, Acharya Nagarjuna University, Guntur-522510, AP*

<sup>2</sup>*Research Fellow in Health Sciences, INTI International University, 71800*

*Nilai, Malaysia & Shinawatra University, Pathum Thani 12160, Thailand*

*E-mail : dr.b.haribabu@gmail.com*

The 3-(3-(Phenylamino)acryloyl)-2H-chromen-2-one scaffolds are widely found in natural products, pharmaceuticals, agrochemicals, and advanced materials. Due to their conjugated electron-donating amino and electron-withdrawing carbonyl groups across the C=C bond, enaminones exhibit unique reactivity and have become valuable building blocks in organic and medicinal chemistry. Brominated derivatives, though known in nature and pharmaceuticals, remain synthetically challenging, especially when involving an enaminone core.

In this study, we report a simple and efficient methodology for the bromination of (E)-3-(3-(phenylamino)acryloyl)-2H-chromen-2-one using N-bromosuccinimide (NBS) to yield the corresponding (Z)-bromo derivatives. The precursor was synthesized from 1-(3-coumarinyl)-3-dimethylamino-2-propen-1-one using (±)-10-camphorsulfonic acid (CSA) as a catalyst, as established in our earlier work. The developed method provides high yields under mild conditions and allows structural variation at the phenyl moiety, expanding the synthetic utility of this scaffold. The present approach offers a versatile route for generating a diverse library of brominated enaminone-based coumarin derivatives with potential applications in drug discovery and materials chemistry.

## **OO-18 : Design and Synthesis of 5-Membered Heterocyclic Hybrids using Conventional and Microwave-promoted Greener Approach**

**Glanish Jude Martis and Santosh L. Gaonkar\***

*Department of Chemistry, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal 576104, Karnataka*

*E-mail: glanish.mitmpl2024@learner.manipal.edu; sl.gaonkar@manipal.edu*

Five-membered heterocyclic compounds are of major interest with respect to their various modes and methods of synthesis. Presently, green approaches have been fascinating tools for the synthesis of such small-organic heterocyclic hybrids. Among them, microwave-assisted organic synthetic protocols have been instrumental in their production. Likewise, the synthetic strategies for the development of such heterocycles were carried out both using microwave as well the conventional/traditional mode of synthesis. Computational studies aid greater assistance for the validation of the synthesized compounds apart from their characterization techniques using FT-IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and mass spectrometry. Molecular docking studies prevail better comfort for the structural properties and possibilities of novel outcomes. Therefore, we herein present few interesting five-membered heterocyclic compounds with their synthetic methods including conventional and microwave-assisted organic synthesis.

## **OO-19 : Highly Efficient Green Synthesis of Novel tetrahydrobenzo[b]thiophene-3-carboxylate Derivatives via Cu-Catalyzed Click Chemistry in Ionic Liquids: A Novel Sonochemical Approach of Synthesis, Biological Evaluation, and Computational Insights**

**Sunita Kurahatti and Rajesh G. Kalkhambkar\***

*Department of Chemistry, Karnatak University's Karnatak Science College, Dharwad, Karnataka 580001*

*E-mail : kurahattisunita@gmail.com*

A series of novel tetrahydrobenzo[b]thiophene-3-carboxylate derivatives were synthesized efficiently via copper catalysed azide-alkyne cycloaddition in an ionic liquid medium under ultrasonication at 50/ °C in 3/ h. The methodology combines mild reaction conditions with excellent atom economy and low waste generation. The green solvent ionic liquid could be recycled over multiple cycles (up to 7) without significant loss of efficiency, demonstrating its potential as a green and sustainable reaction medium. To complement the experimental findings, density functional theory (DFT) calculations

were performed to probe the electronic properties, while molecular docking studies provided insights into the binding interactions with relevant biological targets. Collectively, this study demonstrates a practical, sustainable, and versatile approach for accessing tetrahydrobenzo[b]thiophene-3-carboxylate based scaffolds with potential biomedical applications.

### **OO-20 : Synthesis, Docking Studies and Anti-ulcer Activity of Novel 2-(4,5,6,7-Tetrahydro-1H-indazol-3-yl)-1,3,4-oxadiazole Derivatives**

**Ranjith Kumar K. and C.S. Chidan Kumar**

*Department of Chemistry, Vidya Vikas Institute of Engineering and Technology, Visvesvaraya Technological University, Mysuru, Karnataka  
E-mail : ranjithgaani@gmail.com; chidankumar@gmail.com*

The synthesis of novel tetrahydro-1H-indazol-3-yl)-1,3,4-oxadiazoleactive scaffolds was strategically combined into a single molecular framework to enhance the potency, selectivity, and overall bioactivity of the resulting compounds. These compounds were evaluated for their anti-ulcer potential using established in vitro experimental models. In parallel, molecular docking studies were conducted to investigate the binding interactions of the compounds with key gastric ulcer-related biological targets, such as H<sup>+</sup>/K<sup>+</sup> ATPase. The results revealed favourable binding affinities and critical interactions, supporting the biological relevance of the synthesised molecules. These findings suggest that tetrahydro-1H-indazol-3-yl)-1,3,4-oxadiazoleactive hybrids hold promise as potential anti-ulcer therapeutic agents.

### **OO-21 : Design, Synthesis, Characterization of Novel Coumarin Based Heterocyclic Compounds and Evaluation of Their Antimicrobial Activity**

**B. Vijaya Lakshmi<sup>1</sup>, D. Ashok<sup>2\*</sup> and M. Sarasija<sup>3</sup>**

<sup>1</sup>*Department of Chemistry, TSWRDCW, Mahabubnagar, Telangana, 509001*

<sup>2</sup>*Department of Chemistry, Jawaharlal Nehru Technological University, Hyderabad-500 007*

<sup>3</sup>*Department of Chemistry, Sathavahana University, Karimnagar, Telangana, 505 001*

*E-mail : tswrdcmbnrvp@gmail.com*

The flavonoid compounds are a group of natural products found in fruits, vegetables, nuts, seeds and flowers as well as in teas and are important constituent of human diet. They have been demonstrated to possess antioxidant, antihypertensive, antiallergic, antinociceptive, trypsin inhibitors, plant growth regulator, antibacterial and antifungal activities. The compounds that contain the chromone skeleton (4H-

benzopyran-4-one) (flavones and chromones) are widely spread in nature, and they are part of the flavonoid family. Coumarins fused with other heterocycles are known to have interesting biological and photodynamic properties which, in turn, have encouraged research with regard to procedures for the preparation of families of these compounds. Thus a number of methodologies have been reported for the synthesis of various 3,4-, 6,7- and 7,8-fused furo- and pyranocoumarins. Some members belonging to these two families have shown useful levels of biological activities. On the other hand, very little information is known about medium ring oxacycle fused coumarins which may, in part, be due to lack of general methods for the synthesis of such ring systems. In recent years, ring-closing metathesis (RCM) has emerged as a valuable tool for the construction of various carbocyclic and heterocyclic ring systems especially for medium to large rings.

Environmental pressure to reduce waste and reuse materials has driven studies into 'Green' chemistry. Chemical and pharmaceutical industries are always under pressure to develop more environmentally friendly organic reaction methodologies using nonhazardous catalysis. Microwave irradiation is used for a variety of organic reactions due to short reaction time, cleaner reactions, easier work-up and better yield.

Encouraged by the pharmacological activities of flavanoids we wish to report some new analogs of flavanoids and Macromolecules by simple and convenient microwave irradiation method. All the synthesized compounds were characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, FT-IR, Mass and elemental analysis. All the synthesized compounds screened for their biological activity.

## **OO-22 : Synthesis and Characterization of Nickel Oxide (NiO) Nanoparticles for Various Applications in Organic Reactions**

**Chidananda Murthy B. and H.V. Jayaprakash\***

<sup>1</sup>*Department of Chemistry, Sri Siddhartha Institute of Technology, Maralur, Tumakuru*

*Sri Siddhartha Academy of Higher Education (SSAHE), Agalakote, Tumakuru-572105, Karnataka, India,*

<sup>2</sup>*Department of Chemistry, Siddaganga Institute of Technology, B.H. Road, Tumakuru-572103, Karnataka*

<sup>\*</sup>*E-mail : jpvpsb@gmail.com*

Nickel oxide (NiO) nanoparticles are commonly synthesized by simple, cost-effective chemical methods such as co-precipitation at room temperature, often using nickel salts (e.g., nickel chloride or



nickel nitrate) and ammonia as starting materials. The process typically involves precipitation of nickel hydroxide, followed by filtration, drying and calcination at temperatures around 300°C to 600°C to form NiO nanoparticles. Characterization techniques include X-ray diffraction (XRD) to confirm crystal structure and size, scanning electron microscopy (SEM) and transmission electron microscopy (TEM) to observe particle morphology and size distribution, Fourier-transform infrared spectroscopy (FTIR) for identifying chemical bonds, energydispersive X-ray spectroscopy (EDX) for elemental composition, and UV-Vis spectroscopy for optical properties.

NiO nanoparticles synthesized this way tend to form spherical particles with sizes in the nanometer to micrometer range and exhibit a crystalline structure with a molecular ratio of Ni to O close to 1:1. Due to their favorable properties such as high surface area, stability, and catalytic activity, NiO nanoparticles are widely applied as catalysts in various organic reactions including photocatalytic degradation of dyes and organic pollutants, hydrogenation reactions, and other environmentally relevant transformations.

### **OO-23 : A Sustainable Waste Plastic Valorisation: Conversion of Discarded Polyurethane into Active Micro-Cleaner using DES System**

**Prithvi M. Bhat, Ashok Shrishail Maraddi and S. K. Nataraj\***

*Centre for Nano and Material Sciences, Jain University, Jain Global Campus, Bengaluru-562112, Karnataka*

*\*E-mail : sk.nataraj@jainuniversity.ac.in; sk.nata@gmail.com*

Discarded or waste plastic in the environment can alter health of habitats and natural processes, severely impacting ecosystems, food production capabilities, people's livelihoods, and social well-being. Plastics constitute a major material group with a global production of approximately 368 million metric tons per year. Among them, polyurethane (PU) is a flexible substance with a wide range of applications in daily life and offers adaptability, toughness, and affordability resulted in rapidly increasing demand worldwide. On the contrary, recycling of PU is still limited, and more research and development are needed to improve the efficiency and effectiveness of PU recycling and up cycling. Herein, we demonstrated a sustainable and eco-friendly conversion of waste PU into useful active microcleaners via deep eutectic solvent (DES) assisted solvothermal process. In this process, a greener solvent system containing choline chloride and ferric chloride which acts as solvent and catalyse PU foam into form valuable carbonaceous products under solvothermal condition was established. The prepared PU derived carbon (PUC) were characterized using suitable analytical techniques to understand their physicochemical properties and used for adsorption of variety of contaminants such as malachite green, methylene blue, and a

pharmaceutical ciprofloxacin molecule. Further, PUC successfully demonstrated as Fenton-like catalyst and exhibited excellent recyclability efficiency (>80%) even after 5th cycle which shows potential of the material in sustainable wastewater treatment.

## **OO-24 : Advancing Polymer Membrane Performance through 2D Molybdenum MXene Integration for High-Flux Water Purification and Contaminant Removal**

**P. Satishkumar<sup>1</sup>, Arun M. Isloor<sup>1\*</sup> and Ramin Farnood<sup>2</sup>**

<sup>1</sup>Membrane and Separation Technology Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, 575 025 Mangalore

<sup>2</sup>Department of Chemical Engineering and Applied Chemistry, University of Toronto, M5R OA3, Toronto, Canada

E-mail : isloor@yahoo.com

MXenes, a promising class of two-dimensional materials, have garnered significant attention owing to their rich polar surface terminations and excellent chemical compatibility. In this study, molybdenum-based MXene ( $\text{Mo}_3\text{C}_2\text{T}_x$ , where T represents surface groups such as  $-\text{OH}$  and  $-\text{F}$ ) was successfully synthesized by etching the aluminum layer from  $\text{Mo}_3\text{AlC}_2$  and subsequently incorporated into a polyphenylsulfone (PPSU) matrix to develop a novel mixed matrix membrane. The integration of highly hydrophilic  $\text{Mo}_3\text{C}_2\text{T}_x$  nanosheets into the PPSU matrix remarkably enhanced the water permeability, achieving a maximum flux of  $290 \text{ L m}^{-2} \text{ h}^{-1}$ —over 300% higher than that of the pristine PPSU membrane. Contact angle analysis confirmed improved surface hydrophilicity with increasing MXene loading. The optimized  $\text{Mo}_3\text{C}_2\text{T}_x$ -PPSU membrane exhibited excellent antifouling performance and high pollutant removal efficiency, achieving removal rates of 98.68% for humic acid, 96.7% for Reactive Black 5, 84.72% for Reactive Orange 16, and 80.2% for tetracycline. Overall, this work demonstrates the potential of  $\text{Mo}_3\text{C}_2\text{T}_x$ -embedded PPSU membranes as efficient and multifunctional materials for advanced wastewater treatment, enabling the effective removal of dyes, antibiotics, and organic contaminants.

## **OO-25 : Synthesis and Antimicrobial Activity of Quinoline-Conjugated Benzimidazole Derivatives**

**Deepali D. Garud and Rasika C. Torane\***

<sup>1</sup>Department of Chemistry, Sir Parashurambhau College, Tilak Road, Pune 411030, (Maharashtra)

E-mail : toranerasika@gmail.com

In recent years, a growing number of pharmaceuticals and natural products are using N-containing heterocyclic compounds as scaffolds.

In this regard, quinolines are a versatile class of nitrogen-containing heterocyclic compounds that shows numerous biological activities. Further, the nitrogen-containing benzimidazole heterocycle is a part of several drug molecules due to its diverse pharmacological activities. On the other hand, the piperaziny ring is medicinally important as it often resist metabolic degradation, contributing to a longer half-life of the drug in the body. Therefore, the synthesis of hybrid molecules containing two or more pharmacophore in a single molecule may exhibit improved biological activity. Therefore, we considered the synthesis of a quinoline molecule containing piperazine and benzimidazole heterocycles. The compound 1 was synthesized from corresponding aniline in four steps.

Our group reported a cobalt nitrate and hydrogen peroxide mediated as simple and efficient synthesis of benzimidazoles.<sup>5</sup> The compound 1 was converted to quinoline-conjugated benzimidazole derivatives 2 by treatment with cobalt nitrate and hydrogen peroxide in DMF at 80 °C. The quinoline-conjugated benzimidazole derivatives 2 were characterized by IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR and Mass spectroscopic analysis. Finally, the antibacterial and antifungal activity of compounds 2 was evaluated and they exhibited promising biological activity. The ongoing advancement of existing strategies is in progress within our team.

## **OO-26 : Biogenic Synthesis of Silver Nanoparticles using Camelus Dromedarius Urine: A Nature-Inspired Approach**

**Arfaj Shaikh<sup>1</sup>, Y.I. Shaikh<sup>1</sup> Viqar S. Shaikh<sup>1</sup>, Arun M. Isloor<sup>2</sup> and Mubashir Rasool Pirzada<sup>3</sup>**

<sup>1</sup>*Department of Chemistry, MCE's Abeda Inamdar Senior College, Camp, Pune (MH)*

<sup>2</sup>*Department of Chemistry, National Institute of Technology, Suratkal, Karnataka*

<sup>3</sup>*Department of School Education, Tarzo, Sopore, Srinagar*

Physiologically processed, biologically active molecules naturally occurring in healthy camel liquid excreta are successfully used to reduce transition metal ions into corresponding metal nanoparticles in a single step through novel synthetic routes. This biological process of reducing metal ions to base metals is simple, cost-effective, incredibly fast, and has been applied globally for the first time. The synthesized nanoparticles exhibit excellent catalytic activities for studied organic transformation reactions. X-ray diffraction analysis of the reaction product confirmed the formation of silver nanoparticles. These synthesized AgNPs demonstrate significant potential for organic

transformations. Additionally, the synthesized nanoparticles show potential biological activity against various microorganisms and possess significant antioxidant activity by neutralizing free radicals. Consequently, their antimicrobial and antioxidant properties suggest promising applications in both medical and veterinary sciences. It is believed that, in the near future, camel urine can be effectively used in the synthesis of transition metal and metal oxide nanomaterials with desired biological properties.

### **OO-27 : Natural Product-Inspired Lawsone–Pyrazine and Curcumin Hybrids Synthesis, Characterization, and Anticancer Studies**

**Khursheed Ahmed**

*MCE Society's Abeda Inamdar Senior College, Advanced Scientific Research Laboratory, Azam Campus, Pune-411001, Maharashtra  
E-mail: khursheedahmed@azamcampus.org*

Turmeric (*Curcuma longa*) and Henna (*Lawsonia inermis*) have a long history of therapeutic application in traditional Asian medicine. Natural product-inspired bioactive hybrids were designed and synthesized to enhance anticancer potential. Lawsone–pyrazine (L1–L12) and curcumin-based (CS1–CS6) hybrids were characterized by high-resolution mass spectrometry (HRMS), infrared spectroscopy (IR), and the  $^1\text{H}$  /  $^{13}\text{C}$  nuclear magnetic resonance (NMR) experiments., supported by density functional theory (DFT) calculations. Molecular docking revealed strong interactions of L7, L8, CS2, and CS3 with breast cancer targets - HER2, PR, and ER via hydrogen bonding and hydrophobic contacts. In silico ADMET and toxicity analyses indicated favorable drug-likeness profiles, with minor deviations such as high intestinal absorption or limited blood-brain barrier permeability. L1 and L7 showed CYP2D6 inhibition. Anti-proliferative evaluation against MCF-7 cells demonstrated potent activity, with IC<sub>50</sub> values of 3.83–8.96  $\mu\text{M}$  for CS2 and CS3 and 5.22–6.75  $\mu\text{M}$  for L7 and L8. Flow cytometry was performed. Structure-activity analysis suggested that bulky electron-donating and bioactive moieties enhance anticancer activity. These hybrids represent promising leads for anticancer drug development.

### **OO-28 : The Astrochemistry Behind the Law of Energy**

**Rekha Lagarkha**

*Department of Chemistry Bundelkhand University Jhansi  
E-mail: rekhabuchem@gmail.com*

Astrochemistry traditionally investigates the molecular composition

and reactions occurring in extraterrestrial environments, yet its principles can also illuminate the energetic interactions between planetary radiations and terrestrial biochemistry. This study proposes a chemical framework for understanding how planetary electromagnetic emissions influence molecular and atomic behaviour within the human body. Each planet emits a characteristic spectrum of electromagnetic frequencies; these radiations, when interacting with Earth's atmosphere and magnetic field, may induce subtle shifts in the vibrational and electronic states of biologically relevant molecules.

At the time of human birth, the combined electromagnetic environment forms a unique energy signature that can be conceptualized as an astrochemical equation governing individual energetic equilibrium. These radiative interactions can potentially modulate electron transfer processes, ionic conductivity, and molecular resonance patterns in the body's biochemical systems. Experimental analogies can be drawn from the influence of charged materials—such as copper-ionized water—on enhancing cellular redox activity and energy metabolism. Similarly, water exposed to lunar radiation may undergo changes in hydrogen bonding networks, influencing hydration dynamics and emotional homeostasis, while the energetic influence of Mercury is hypothesized to correlate with neural signalling and consciousness through modulation of synaptic charge transfer.

By integrating astrochemical principles with molecular energetics and biophysical chemistry, this work advances the concept of a Law of Energy that bridges cosmic radiation, planetary chemistry, and human bioenergetics. This interdisciplinary framework invites further investigation into how extraterrestrial energy fields may influence molecular organization and chemical reactivity within living systems.

## **OO-29 : Structural Elucidation and Computational Insights into Bioactive Heteroaromatic Sulfonamide Analogues**

**K. Jyothi<sup>1\*</sup>, Poornima Hegde<sup>2</sup> and Damodara Naral<sup>3</sup>**

<sup>1</sup>*Department of Chemistry, St Joseph Engineering College Vamanjoor, 575028*

<sup>2</sup>*Expert Pre University College, Mangaluru*

<sup>3</sup>*Alva's Institute of Technology, Moodubidri, Mangaluru*

*E-mail: jyothik@sjec.ac.in; poornima.upadyaya@gmail.com; dnaral@gmail.com*

A series of bioactive heteroaromatic sulfonamide analogues has been synthesized and systematically characterized to investigate their structural, electronic, and biological properties. The synthesized compounds were confirmed through FTIR, UV-Vis, <sup>1</sup>H NMR, and <sup>13</sup>C NMR spectroscopic analyses, complemented by elemental and, where available, single-crystal X-ray diffraction studies. Density Functional

Theory (DFT) calculations at the B3LYP/6-311G(d,p) level were performed to optimize molecular geometries and evaluate frontier molecular orbitals, electronic density distribution, and reactivity descriptors. The highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) and their associated parameters were computed to explain intra-molecular charge transfer and global reactivity properties of the compounds with the level of theory. The compounds were further evaluated for their anti-inflammatory activity, and several derivatives exhibited notable inhibition compared to standard drugs, indicating their potential pharmacological relevance. The combined experimental, computational, and biological approach provides valuable insights into the structure–activity relationship of heteroaromatic sulfonamide derivatives as promising anti-inflammatory agents.

### **OO-30 : Synthesis, Biological Evaluation and In Silico Studies of New Class of Triazole-linked Pyrimidine Derivatives**

**Hari K.N.<sup>1,2</sup>, Boja Poojary<sup>1\*</sup>, Vinuta Kamat<sup>3</sup>, S.B. Gowdar<sup>4</sup> and Mahesh Akki<sup>5</sup>**

<sup>1</sup>*Department of Chemistry, Mangalore University, Mangalagangothri-574199, Karnataka*

<sup>2</sup>*Rallis India Limited (A TATA Enterprise), Byregowda Industrial estate, Hegganahalli, Peenya, Bengaluru-560091 Karnataka*

<sup>3</sup>*Dayananda Sagar college of engineering, Shavige Malleshwara Hills, 91st Main Rd, 1st Stage, Kumaraswamy Layout, Bengaluru- 560078, Karnataka*

<sup>4</sup>*Department of Plant Pathology, College of Agriculture, Gangavathi-58322, Karnataka*

<sup>5</sup>*Department of Chemistry, Smt. Kamala and Sri Venkappa M. Agadi College of Engineering and Technology, Lakshmeshwar-582116, Karnataka*

<sup>\*</sup>*E-mail : poojaryboja@gmail.com*

A new class of triazole-linked pyrimidine derivatives (25a–n) was rationally designed, synthesized, and characterized to explore their antifungal potential. The structures of all synthesized compounds were confirmed using FT-IR, <sup>1</sup>H/<sup>13</sup>C NMR, LC-MS, and their purity (96–99%) was verified by HPLC. The antifungal activity of these hybrids was evaluated against *Fusarium oxysporum* and *Colletotrichum* sp. at 200 ppm. Notably, compounds 25a, 25g, and 25n exhibited complete (100%) inhibition of *F. oxysporum*, while compounds 25i, 25j, and 25n showed strong inhibition against *Colletotrichum* sp., with 25j achieving 100% inhibition, comparable to the standard fungicide.

Molecular docking studies performed against lanosterol 14- $\alpha$ -demethylase revealed favourable binding affinities (–8.9 to –8.2 kcal/mol), supporting the observed biological activity. Strong hydrogen-bonding,  $\pi$ -stacking, and hydrophobic interactions were identified for



the most active molecules, correlating well with their in vitro performance. Overall, these findings highlight triazole-linked pyrimidine derivatives as promising lead scaffolds for developing potent antifungal agents.

### **OO-31 : High-Efficiency Arsenic (V) Removal Using Aluminium Oxide-Integrated PES Hollow Fiber Membranes via Ultrafiltration**

**Mruthyunjaya Swamy D.<sup>1</sup>, Arun M. Isloor<sup>1\*</sup>, Muttanna Venkatesh<sup>1</sup> and Vijayendra Shetti<sup>2</sup>**

*<sup>1</sup>Membrane and Separation Technology Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, 575 025, Mangalore  
E-mail : isloor@yahoo.com*

This study integrates nanotechnology and membrane technology to address the critical issue of water scarcity by transforming polluted water into safe, potable water. In this research, Polyethersulfone (PES) hollow fiber membranes (HFMs), both with and without nanoparticles (NPs), were developed using the dry-wet spinning technique. These membranes were employed to remove arsenic [As(V)] ions from wastewater. To evaluate the membranes and the nanoparticles, several characterization techniques were used, including scanning electron microscopy (SEM), atomic force microscopy (AFM), and Fourier transform infrared spectroscopy (FTIR). These methods helped to analyse the morphology, surface roughness, and chemical functional groups of the materials. The findings revealed a notable enhancement in arsenic removal efficiency, with the M-2 membrane achieving a removal rate of 79.23% and the highest flux of 26.7 L/m<sup>2</sup>/h. In contrast, the standard M-0 membrane demonstrated a removal rate of 65% and a flux of 18 L/m<sup>2</sup>/h. This study underscores promising potential of these membranes in advancing water purification technologies.

### **OO-CYSA-01 : COF/NiCoFe LDH Incorporated PES Hollow Fiber Ultrafiltration Membrane for Agrochemical and Dye Separation from Wastewater**

**Haritha Pallot and Arun M. Isloor<sup>\*</sup>**

*Membrane and Separation Technology Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, Mangalore, Karnataka-575025  
E-mail : isloor@yahoo.com*

The contamination of water bodies with agrochemicals and textile dyes poses a significant challenge to environmental integrity. In this work, COF/NiCoFe layered double hydroxide (LDH) was synthesized



by the hydrothermal method with a molar ratio of 2:1:1 of nitrates of Ni, Co, and Fe metals. For the first time, COF/NiCoFe LDH incorporated hollow fiber membranes were fabricated and employed for the separation of hazardous agrochemicals and dyes from wastewater. The incorporation of hydrophilic COF/NiCoFe LDH into polyether sulfone (PES) membranes improved the pure water flux from 75.41 Lm<sup>-2</sup>h<sup>-1</sup> to 130.85 Lm<sup>-2</sup>h<sup>-1</sup>. The MLC-2 membrane revealed a good antifouling nature with a flux recovery ratio of 68.8 %. The optimized membrane (MLC-2) exhibited 92.6 % and 49.1 % rejection of chlorpyrifos and 2,4-dichlorophenoxy acetic acid, respectively, while the neat membrane showed 69.9 % and 42.5 %. In case of dyes, the MLC-2 showed rejection of 99.2 % for Crystal Violet and 84.9 % for Reactive Orange 16, whereas the values for pristine membrane were 74.8 % and 69.8 % respectively. Therefore, the COF/NiCoFe LDH-PES hollow fiber membranes can potentially be used for the removal of agrochemicals and textile dyes from wastewater.

## **OO-CYSA-02 : Development of Electron Donor-Acceptor Fluorophores Incorporating 2-(2-(tert-butyl)-6-methyl-4h-pyran-4-ylidene)Malononitrile Frameworks for Sensing and Biological Studies**

**Gummadi Leela Prabha Anisha and Ravi Kumar Kanaparthi\***

*Department of Chemistry, Central University of Kerala, Tejaswini Hills, Periyar, Kasaragod, Kerala, 671316*

*E-mail : anisha.pch072203@cukerala.ac.in; rkchem@cukerala.ac.in*

Organic molecules with delocalized  $\pi$ -electrons are desirable candidates for developing functional materials for various applications. Organic  $\pi$ -conjugated molecules are inexpensive to synthesize, and their structure-property relationship can be customized to our particular interests, making them ideal candidates in material science. To develop two new fluorescent sensors namely, AP-1 & AP-2 based on 2-(2-methyl-4H-chromen-4-ylidene)malononitrile and 2-(2-(tert-butyl)-6-methyl-4H-pyran-4-ylidene)malononitrile acceptors and conjugated  $\delta$ -systems is 4-(bis(pyridin-2-ylmethyl)amino)benzaldehyde as electron donors shows a turn ON-OFF fluorescence sensor for Zn(II) based on an intramolecular charge-transfer (ICT) mechanism. AP-1 and AP-2 were synthesized by following well-known chemical reactions such as Vilsmeier-Haack formylation and Knoevenagel condensation. And also, AP-1 & AP-2 bind with zinc metal chelation. Since zinc has more biological importance. Furthermore, these molecules have been characterised using FT-IR, TGA, HRMS, and <sup>1</sup>H-NMR spectroscopy. Photophysical properties were studied systematically using a UV-visible spectrophotometer and spectrofluorometer. Results show that the two

molecules are thermally stable and exhibit strong absorption characteristics in the UV-visible region (250-650nm) and strong fluorescence characteristics in the 400-800nm region in various solvents. Further, upon screening for the detection of different metal ions, these molecules sense selectively for Zinc ions. The zinc ion detection is visible to the naked eye.

### **OO-CYSA-03 : Ultrasound-assisted Ring Opening of Epoxides in HFIP: THF: Synthesis, Characterization, Computational Studies and Molecular Docking of Novel 2 Hydroxy Dithiocarbamates**

**Amit Patel, Vishal Prasad Sharma and Ashish Kumar Tewari\***

*Department of Chemistry, Banaras Hindu University, Varanasi-221005*

*\*E-mail : ashishtewarichem@gmail.com*

Under the influence of ultrasonic irradiation, pyridazinone, triazinone, or phthalimide containing 2 hydroxy dithiocarbamates, a biologically relevant novel organo-sulfur compound, was synthesized. Detailed characterizations, computational, and molecular docking studies are being investigated. Molecular interactions were studied using 3D Hirshfeld surfaces and corresponding 2D fingerprint plots. Theoretical (DFT) studies on the molecular structure, HOMO, LUMO, and quantum chemical descriptors were performed at the B3LYP/ 6-311++G(d,p) level of theory. At the same time, the interaction energy was computed using the B3LYP/6-31G (d,p) level of theory. The FMO study revealed that molecules 4a and 4p in the gas phase have 3.545 eV and 3.263 eV HOMO-LUMO energy gaps, respectively, and they are hence kinetically stable. Quantum chemical calculations confirm the electrophilic character of compounds 4a and 4p, as the molecule is stable and highly electrophilic. The interactions of 2 hydroxy dithiocarbamate derivatives (4a-4t) with the ligand-binding site of the target COX-2 (cyclooxygenase-2) enzyme were investigated using in-silico molecular docking experiments. Compared to the standard medicine celecoxib, the results showed that most synthesized derivatives had better glide scores and interaction. The docking study of all the synthesized compounds revealed that compounds 4a, 4e, and 4o interact well with the COX-2 enzyme as anti-inflammatory drugs. Molecular dynamic simulation was utilized to validate the docking study and explore the stable binding site and interaction of compound 4o, which is the most potent. The findings indicated that compound 4o exhibited better stability and interaction when compared to the reference drug.

## **OO-CYSA-04 : Ti-PolyMOF-Induced Polysulfone Membranes for Heavy Metal Ion Rejection**

**Shyam S. Desai<sup>1,2</sup>, Kiran Thabaj<sup>1</sup>, Shridhar Malladi<sup>3</sup>, Mahesh Padaki<sup>4</sup>, Usha Nellur<sup>4</sup>, Charushil<sup>1</sup> and V. Balikai<sup>1,2</sup>**

<sup>1</sup>*Department of Chemistry, Centre for Nanoscience and Nanotechnology, KLS Gogte Institute of Technology, Belagavi, Karnataka*

<sup>2</sup>*Department of Chemistry, SKE's Govindram Seksaria Science College, Belagavi 590006, Karnataka*

<sup>3</sup>*Department of Chemistry, Anuvartik Mirji Bharatesh Institute of Technology, Belagavi, Karnataka*

<sup>4</sup>*Centre of Nano and Material Science, Jain (Deemed-to-be University), Jain Global Campus, Kanakapura, Bengaluru 562112, Karnataka*

*E-mail : desaishyam22@gmail.com*

Wastewater remediation remains a critical global concern, despite numerous technological advancements and accomplishments. Nanoparticle-induced membrane technology has gained tremendous attention for removing heavy metal ions from wastewater compared to many other known methods, mainly due to its affordable capital cost and low energy consumption. Polymerbased metal-organic frameworks (polyMOFs) and their composite membranes are reported in this work. Comprehensive characterization of the polyMOF and composite membranes is conducted by using FTIR, XRD, TGA, tensile strength, contact angle, and SEM techniques. The Ti-polyMOF/PSf composite membrane performance towards metal ion filtration was carried out. Rejection of about 98% of Cd<sup>2+</sup>, 97.86% of Pb<sup>2+</sup> and 91.42% of Cr<sup>2O7</sup><sup>2-</sup> was achieved using deadend filtration technique. Additionally, membranes demonstrated outstanding antifouling properties and achieved an 83% flux recovery ratio with a total fouling of at least 18% for 100 ppm of Bovine Serum Albumin as the foulant. Water uptake and pH-dependent studies for the membranes are also reported.

## **OO-CYSA-05 : Energy-Efficient and Eco-Conscious Elimination of Microplastics and Toxic Contaminants Using 3D MOF Integrated Hollow Fiber Membrane Via Ultrafiltration**

**Muttanna Venkatesh<sup>1</sup>, Arun M. Isloor<sup>1\*</sup> and Ramin Farnood<sup>2</sup>**

<sup>1</sup>*Membrane and Separation Technology Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, 575 025, Mangalore*

<sup>2</sup>*Department of Chemical Engineering and Applied Chemistry, University of Toronto, M5R,*

*E-mail : isloor@yahoo.com*

The rapid build-up of hazardous pollutants from industrialization has led to contamination of aquatic ecosystems with microplastics

(MPs), dyes, and heavy metals, creating environmental and public health risks that necessitate effective advanced water purification methods. Traditional techniques are often inefficient, expensive, and cause secondary pollution, emphasizing the need for advanced membrane-based treatments. In this study, an innovative Polyethersulfone hollow fiber membrane (HFM) embedded with a ZIF-8@NH<sub>2</sub>-MIL125(Ti) Metal-Organic Framework (MOF) composite is presented for efficient water purification. The synergistic effects of ZIF-8 and NH<sub>2</sub>-MIL125(Ti) MOFs synthesis were confirmed through various physicochemical characterizations. Additional tests confirm the successful fabrication of HFM by Field Emission Scanning Electron Microscopy, Contact Angle Measurement, Atomic Force Microscopy, a Universal Testing Machine, and Membrane Zeta Potential analysis. Membranes showed improved performance in the membranes' hydrophilicity, Pure Water Flux (PWF), Anti-Fouling Ability, and rejection efficacy. Whereas, PWF increased from 90.49 L·m<sup>-2</sup>·h<sup>-1</sup> (ZM-0) to 159.07 L·m<sup>-2</sup>·h<sup>-1</sup> (ZM-2) membrane, with rejection efficiencies of 36.3% and 97% for P(St-co-MMA) MPs, 67.66% and 99.5% for Crystal Violet, 77% and 86% for Reactive Orange 16, 65.4% and 87% for Pb<sup>2+</sup>, and 57.9% and 68.9% for Hg<sup>2+</sup>, respectively. This research demonstrates that an energy-efficient MOF-engineered HFM offers a sustainable solution for advanced filtration methods.

## **OO-CYSA-06 : Design and Efficient Synthesis of a Key Starting Material of Ciprofloxacin Antibiotic**

**Sushama Kadam<sup>1</sup> and Nilesh Paymode<sup>2</sup>**

<sup>1</sup>*Department of Chemistry, DGM's Hon'ble B.J. Arts, Commerce & Science College, Ale, Junnar, Pune, Maharashtra*

<sup>2</sup>*Chemistry Research Centre, Rayat Shikshan Sanstha's Annasaheb Awate Arts, Commerce & Hutatma Babu Genu Science College, Manchar, Pune, Maharashtra*  
E-mail : sushmaarjun522@gmail.com

In this research article we tried to disclose a preparation method of 2, 4-dichloro-5-fluorobenzoyl chloride core structure is the essential pharmacophore of Ciprofloxacin and related fluoroquinolone antibiotics. Ciprofloxacin is a fluoroquinolone antibiotic used to treat a number of bacterial infections. The invention adopts 2, 4-dichlorofluorobenzene as a raw material, generates an intermediate 2, 4-dichloro-5-fluorobenzoyl chloride shows colorless to light yellow liquid, stable under inert conditions, moisture sensitive has boiling point approx. 245 °C. Successive Friedel-Craft reaction provides the targeted compound. During step-1, the Dimer formation observed which can lead to a final product compound through hydrolysis, oxidation and F. C. acylation, and has the overall yield of more than 70-80%. It was isolated by high vacuum distillation at 190°C and solid material dimer

was isolated via filtration method. This optimized synthesis presents a significant advancement for the industrial-scale production of KSM of Ciprofloxacin and a versatile platform for the synthesis of novel fluoroquinolone derivatives. The method demonstrates exceptional scalability and provides a high-purity product, as confirmed by HPLC and NMR spectroscopy. More advancement and yield improvement can be done by flow chemistry technology. This technology allows a continuous flow of reagent to be introduced at various points along a process stream, enabling interaction under highly controlled conditions. Flow system allows high through put chemistry to take place, often employing immobilized reagents or catalysts.

## **OO-CYSA-07 : Quantitative Determination of Strength of Borane Reagents via No-D and PULCON NMR**

**Shrikant A. Shete<sup>1,2</sup>, Prashantha Kamath<sup>1</sup>, Sujit K. Ghorai<sup>1,2</sup> and Bhanu N. Manjunath<sup>1,2\*</sup>**

<sup>1</sup>*Syngenta Biosciences Pvt. Ltd., Santa Monica Works, Corlim, Ilhas, Goa-403110*

<sup>2</sup>*School of Chemical Sciences, Goa university, Taleigao Plateau, Goa-403206*

Borane and borohydride reagents are indispensable tools across a wide spectrum of chemical disciplines, serving critical functions in organic synthesis, medicinal chemistry, materials science, and even food chemistry. Due to their high reactivity and pyrophoric characteristics, borane poses significant operational challenges that disrupt routine analytical procedures and raise serious safety concerns. These limitations hinder both the evolution of analytical techniques and their broader industrial adoption. Consequently, advancing novel analytical approaches that harmonize stringent safety protocols with precise analytical performance stands as a critical priority in modern borane chemistry research.

A wide array of analytical techniques has been established for the detection and quantification of borane reagents, with methods such as hydrogen evolution and titration among the most commonly employed. Conventional quantification of boron reagents relies on complex analytical techniques, including gas burette methodology, iodometric titration, and titrimetric approaches based on acid-base or redox chemistry. Therefore, there is a need for simpler and easy to perform analytical technique for the determination of strength of boranes reagents. In this study, we present an analytical protocol that enables quantitative determination of commercial borane and borohydride reagents solution (in THF & Hexane). The approach synergistically integrates two NMR techniques, No-D (No deuterium) and PULCON NMR (Pulse Length-based Concentration Determination), which gives insight into quantitative determination of reagent and identification of impurities. Proposed method has been validated and tested on seven

different borane and borohydride reagents, yielding well-correlated results.

## **OO-CYSA-08 : Molecular Docking Study of Quinoxalinone-based Ligands Against HDAC1 Inhibitors**

**Shumaila Nafees and Neeraj Kumar Mishra\***

*Department of Chemistry, University of Lucknow, Lucknow-226007, U.P.*

*\*E-mail : neerajchemistry@gmail.com*

The identification of quinoxalinone-based inhibitors against zinc-dependent HDAC1 metalloenzyme is crucial for the discovery of new therapeutic agents as a key epigenetic regulator implicated in cancer and other proliferative disorders. In this work, molecular docking was done to evaluate the binding affinity and interaction profiles of a quinoxalinone, and its seven already reported derivatives. Also, three-dimensional structures of the ligands were optimized using Chem3D 19.0. and molecular docking was executed by using LeadIT software. From the docking results, it can be concluded that these ligands exhibit favourable binding characteristics within the enzyme's catalytic pocket. The 2D interaction visualizations provided by Discovery Studio revealed key binding modes and interaction fingerprints for each ligand. Common hydrogen bonding residues such as His39, Asn40, and Arg36 were consistently observed across multiple ligands. Aromatic interactions were particularly prominent with Tyr15, Phe252, Phe205, and Phe150, indicating  $\pi$ - $\pi$  stacking and  $\pi$ -sigma contacts that reinforced ligand orientation within the active site. Introducing zinc-binding groups may improve their effectiveness. These findings support the development of optimized quinoxalinone-based HDAC1 inhibitors for cancer treatment. The study further explains the solid basis for the logical development of quinoxalinone-based HDAC1 inhibitors that are optimized. They also stimulate additional research into these scaffolds as possible epigenetic modulators that could be used therapeutically in the development of anticancer drugs which I will explain in my oral presentation.

## **OP-01 : Synthesis, Structural Characterization, and Antioxidant Evaluation of Para-Substituted Phenyl-Benzimidazolylthio-4-Hydroxyquinolin-2(1H)-ones: Insights from Molecular Docking and DFT Analysis**

**Amrutha M. and Yadav D. Bodke\***

*Department of PG Studies and Research in Chemistry, Jnanasahyadri,*

*Kuvempu University, Shankaraghatta, Karnataka 577451*

*\*E-mail : ydbodke@gmail.com; amrutham.bdvt@gmail.com*

In this work, we report the synthesis of a series of 3-[(1H-1,3-benzimidazol-2-yl)thio(4-R-phenyl)methyl]-4-hydroxyquinolin-2(1H)-ones



and their structural characterization by FT-IR,  $^1\text{H}$  and  $^{13}\text{C}$  NMR, and high-resolution mass spectrometry. The compounds were obtained through nucleophilic substitution of 2-mercaptobenzimidazole with para-substituted benzaldehydes, followed by coupling to the 4-hydroxyquinolinone core. Antioxidant potential was assessed through DPPH radical scavenging assay. These compounds displayed prominent activities, corresponding to substituent-dependent electronic effects. Molecular docking studies revealed stable binding conformations within antioxidant-relevant protein targets, with key interactions arising from hydrogen bonding and  $\pi$ - $\pi$  stacking. Furthermore, density functional theory [DFT, B3LYP/6-31G+(d,p)] calculations provided insights into frontier molecular orbital distributions, band gaps, and electronic parameters that rationalize the observed structure-activity relationships. The combined experimental and computational findings establish Phenyl-substituted benzimidazole-sulfanyl-hydroxyquinolin-2(1H)-one derivatives as promising antioxidant scaffolds and highlight the impact of substituent electronic properties on biological efficacy.

## **OP-02 : Sustainable Biodiesel Production from Anamitra Cocculus Seed Oil using Ni-Co Ferrite Catalyst: Kinetic and Thermodynamic Evaluation**

**Surekha Kademani and Kariyappa S. Katagi\***

*<sup>1</sup>Research centre, Department of Chemistry, Karnatak University's Karnatak Science College, Dharwad-580001, Karnataka  
E-mail: surekhakademani@gmail.com; kskatagi69@gmail.com\**

In this study, a magnetic Ni-Co Ferrite nanocatalyst was synthesized via the sol-gel method and applied for biodiesel production from Anamitra cocculus seed oil through transesterification. The catalyst was characterized using XRD, FT-IR, SEM, EDX, and VSM analyses. VSM results confirmed its superparamagnetic behaviour at room temperature with a saturation magnetization ( $M_s$ ) of 21.78 emu/g, enabling easy recovery using an external magnet. Optimal transesterification conditions were a methanol-to-oil molar ratio of 8:1, 65/ °C temperature, and 4 wt% catalyst loading, yielding 94.8% biodiesel. The produced biodiesel was characterized by FTIR,  $^1\text{H}$  NMR, and  $^{13}\text{C}$  NMR, and its thermal stability was validated via TGA. The transesterification reaction showed pseudo-first-order kinetics with rate constants ranging from 0.0154 to 0.0167  $\text{min}^{-1}$ , with an activation energy ( $E_a$ ) of 3.69 kJ/mol and frequency factor ( $A$ ) of 16.44  $\text{min}^{-1}$ . Thermodynamic studies indicate that the reaction is endothermic and non-spontaneous. The fuel properties of the biodiesel complied with ASTM and EN standards, confirming its suitability for commercialization.



### **OP-03 : Structural Insights, BSA Binding, and Anticancer Evaluation of 2,6-Dipyrazinylpyridines: An Experimental and Theoretical Study**

**Sreenivasulu Enumula<sup>1,2</sup>, Pranav Tambe<sup>1,2</sup> and Khursheed Ahmed<sup>1,2\*</sup>**

<sup>1</sup>*Department of Chemistry and Post Graduate Research Centre, Abeda Inamdar Senior College, Pune-411001, Maharashtra*

<sup>2</sup>*Advanced Scientific Research Laboratory, Abeda Inamdar Senior College, Pune-411001, Maharashtra.*

Phenyl-(2,6-di-2-pyrazinyl) pyridine derivatives (L1, L2) were synthesized via a one-pot Krohnke-type method from 2-acetylpyrazine and substituted benzaldehydes. Their structures were confirmed using NMR, HRMS, single-crystal X-ray diffraction, and supported by DFT studies. X-ray analysis showed L1 crystallizes in the C2/c space group with C–H $\cdots$ N and  $\pi$ – $\pi$  stacking, while L2 displays C–H $\cdots$ N, N–H $\cdots$  $\pi$  bifurcated, and  $\pi$ – $\pi^*$  interactions. Fluorescence studies with BSA revealed static quenching by L1 ( $K = 5.15 \times 10^4 \text{ mol dm}^{-3}$ ), significant conformational changes, and cytotoxicity against HCT-116 cells.

### **OP-04 : Synthesis of Substituted Coumarins Through Several Methods: A Review**

**Sanjeev Kumar Mishra**

*Department of Chemistry, J.L.N P.G College Etah*

*E-mail: Sanjeevskb@gmail.com\**

Coumarins represent an important class of heterocyclic compounds known for their wide range of biological and pharmacological activities, including antimicrobial, anti-inflammatory, antioxidant, and anticancer properties. The synthesis of substituted coumarins has attracted significant attention due to their diverse applications in medicinal chemistry, perfumery, and material science. Various synthetic approaches have been developed to construct coumarin derivatives efficiently, with the Pechmann condensation, Knoevenagel condensation, and Perkin reaction being the most widely employed methods. In the Pechmann condensation, phenols react with  $\beta$ -ketoesters or malic acid in the presence of acid catalysts to yield coumarins under mild conditions. The Knoevenagel condensation, involving salicylaldehydes and active methylene compounds, offers a versatile route for introducing diverse substituents at the 3- and 4-positions of the coumarin ring. Additionally, methods such as the Wittig reaction, Baylis–Hillman reaction, and metal-catalyzed cyclization have been explored to achieve regioselective and functionalized coumarins. Recent advancements in green chemistry have further improved the sustainability of these syntheses, utilizing solvent-free conditions, microwave irradiation, and ionic liquids as

eco-friendly alternatives. These innovations not only enhance reaction efficiency but also reduce environmental impact.

### **OP-05 : Solid State Kinetics of Hg (I) Complex Derived from Schiff base of 5-Amino-1,2,3,4-Thiatriazole with-Ortho-Methoxybenzaldehyde**

**Ajay Kumar**

*Department of Chemistry, J.L.N College, Dehri-On-Sone (Rohtas)*

Thermal analysis has become an established method in the study of thermal behavior of materials and finds wide applications. The mercury complex (HgLcl<sub>2</sub>) where L is Schiff base derived from 5-Amino [1,2,3,4] Thiatriazole was synthesized by refluxing the Schiff base with mercuric chloride, and gravimetric analysis. The molecular weight was found to be 692.18mg. Thermal analysis was performed using thermogravimetric Analysis (TGA) Which showed Two distinct stages of weight loss, initial loss of ligand moiety and finally two chloride ion. These steps were analyzed to determine kinetic parameters using freeman-Carrole and zasko's modified Doyle method.

The order of reaction for the main decomposition step was formed to be approximately 1 using freemen-Carrole and 1 using zasko's method. The corresponding activation energies were 23.45 kcal/mol and 26 kcal/mol respectively.

The apparent entropy of activation ( $\Delta S^\ddagger$ ) was calculated as -389.343348759 e.u and the frequency factor(Z) was found to be  $2.53705947 \times 10^3 \text{ sec}^{-1}$  These results obtained by different methods were in good agreement and support the reliability of the kinetic model. These findings help in understanding the thermal behaviors and stability of mercury-Schiff base complexes in the solid state.

### **OP-06 : Design, Synthesis and Characterization of N-Substituted Heteroaromatics: DFT-Studies and Sensing Properties**

**Dhanusha K.K.<sup>1</sup> and Vijesh A.M.<sup>1,2\*</sup>**

<sup>1</sup>*PG and Research Department of Chemistry, Government College, Kasaragod, Kannur University, Kerala-671314*

<sup>2</sup>*PG Department of Chemistry, Payyanur College, Payyanur, Kannur University, Kerala-670327*

<sup>\*</sup>*E-mail : dhanukk01@gmail.com, vijeshnambisan82@gmail.com*

Ionic dipole, electrostatic,  $\pi$ - $\pi^*$ , and hydrogen bonding interactions are the driving forces behind the interactions of ions with organic compounds, shaping the field of supramolecular chemistry. These principles guide the creation of host-guest complexes and the

development of selective chemosensors to identify various analytes. Chemosensors have a vital role in both qualitative and quantitative recognition of metal ions and anions due to their vital role in physiology and potential contribution to environmental pollution. Designing and developing selective chemosensors is very significant for the determination of metal ions in various fields. The present investigation includes designing, synthesis, and studies on some schiff bases based N-substituted heterocyclic compounds as new reagents for spectrophotometric determination of aluminum ions. The newly synthesized compounds have been characterized by elemental analyses, IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, and mass spectral studies. The proposed methods will be validated according to ICH guidelines for intended analytical applications. The theoretical analysis of the synthesized chemosensors was studied using DFT calculations. Finally, a live-cell image study of the synthesized fluorescent probes will also be carried out to investigate the cell permeability and its efficiency for selective detection of Al<sup>3+</sup> in living cells.

### **OP-07 : Fabrication, Characterization and Water Purification studies of Modified PES/ Manganese Ferrite Nanocomposite Hollow Fiber Membrane**

**Viji K.<sup>1</sup> and Vijesh A.M.<sup>1,2\*</sup>**

<sup>1</sup>*P.G. and Research Department of Chemistry, Government College, Kasaragod, Kannur University, Kerala- 671123*

<sup>2</sup>*P.G. and Research Department of Chemistry, Payyanur College, Payyanur, Kannur University, Kerala- 670327*

<sup>\*</sup>*E-mail : vijeshnambisan82@gmail.com*

The presence of heavy metals in water has been increasing with the growth of industry, mining and human activities, which causes the environmental pollution primarily water pollution. The heavy metals are non-biodegradable and could be carcinogenic; thus, the presence of heavy metals in drinking water by improper amounts could result in critical health issues to living organisms. Therefore waste water must be treated properly to remove the contaminated heavy metals. Among different purification techniques, membrane based separation technology is most popular for the removal of toxic heavy metals due to its cost effectiveness and ease of fabrication. Hollow fiber membranes are superior to flat sheet membranes in terms of surface area per volume, making them excellent choice for water treatment. The nature and properties of materials used in the fabrication affects the membrane separation efficiency.

Polyether sulfone is one of the most widely used membrane base polymer as it has high mechanical strength, good chemical resistance

and thermal stability. This abstract presents an overview of polyether sulfone (PES) based composite membranes with manganese ferrite nano additives, highlighting their characterization and application in heavy metal removal studies. Phase inversion technique was adopted for the formation of well- defined nanocomposite membranes with enhanced structural and functional properties. Detailed characterization techniques provide insight into the morphology and chemical properties. SEM, water uptake, contact angle, water permeability, porosity, antifouling capabilities and heavy metal rejection experiments were carried out. The incorporation of nano additives significantly enhanced the membrane's efficiency in removing heavy metals, specifically lead (Pb) and Cadmium (Cd). The findings indicated that the additives effectively improve membrane performance without compromising rejection efficiency. The results of such studies will be discussed in this paper.

### **OP-08 : Thiazole-Conjugated Thiazolidinone Derivatives: Synthesis, Characterization, and Pharmacological Assessment for Antimicrobial, Antifungal, and Anticancer Activities**

**Valsaraj V.P.<sup>1,2</sup> and Vijesh A. M.<sup>2,3,\*</sup>**

<sup>1</sup>*Department of Chemistry, Govt. Brennen College, Dharmadam, Thalassery, Kannur University, Kerala-670106*

<sup>2</sup>*P.G. Department of Chemistry, Government College, Kasaragod, Kannur University, Kerala-671123*

<sup>3</sup>*Department of PG Studies and Research in Chemistry, Payyanur College, Payyanur, Kannur University, Kerala-670327*

<sup>\*</sup>*E-mail : vijeshnambisan82@gmail.com*

Thiazolidinone scaffolds are the privileged small molecules with unique properties in medicinal chemistry. Owing to the extraordinary biological profile of these molecules, these are considered as magic moiety in medicinal chemistry research. It exhibits different pharmacological activities such as antibacterial, antitubercular, anti-inflammatory, anticancer, and antiviral. Thiazoles are also promising heterocyclic entity in pharmaceutical field. Incorporation of this small motif in different molecules enhances the bio-availability of the drug candidates. It was noteworthy to mention the applications of clubbed pharmacophore of thiazole and thiazolidinone in medicinal chemistry. Thiazole endowed thiazolidinone derivatives were found to exhibit diverse biological activities such as antimicrobial, antitubercular, anti-inflammatory and anticancer.

Prompted by the pharmacological importance of thiazoles and thiazolidinones, it was contemplated to synthesize some new 2-

aminothiazole endowed arylidene containing thiazolidinone derivatives starting from substituted-2 amino thiazoles via multistep reactions. The newly synthesized compounds were characterised by spectral studies and screened for their antimicrobial and anticancer activities. The results of such studies will be discussed in this paper.

General structure of 2-aminothiazole endowed arylidene containing thiazolidinone derivatives

## **OP-09 : Design and Characterization of Biopolymer Materials**

**Meeta P. Patel, Arati J. Peajapati, H.D. Chaudhari and J.J. Vora**

*Department of Chemistry, Hemchandracharya North Gujarat University, Patan-384265*

*E-mail : meetap2904@gmail.com*

This research focuses on the chemical modification of natural biopolymers to enhance their functional performance and expand their practical applications. Starch, an abundant, biodegradable, and non-toxic biopolymer, was chosen as the primary material. Through targeted chemical modification, new functional groups were incorporated into the starch backbone to improve its physical, chemical, and surface characteristics. The modified starch was systematically characterized using various analytical techniques to assess alterations in molecular structure, particle size, morphology, and surface behavior. The findings confirmed that the modification process was effective, revealing distinct differences compared to native starch. These improvements indicate enhanced stability, solubility, and overall functionality. Such chemically modified biopolymers exhibit significant potential or applications in pharmaceuticals, medicine, food, packaging, and other industrial sectors.

## **OP-10 : Biochemical and Mechanistic Characterization of Enzymes Involved in Gourgerotin Biosynthetic Pathway**

**Dhwani Shah and Nilkamal Mahanta\***

*Department of Chemistry, Indian Institute of Technology Dharwad, Dharwad, Karnataka 580011*

*E-mail : 222051001@iitdh.ac.in*

Natural products and their derivatives serve as sources of antibacterial, antiviral, anticancer, and antifungal drugs. However, the emergence of antimicrobial resistance (AMR) to these proven drug classes is posing a grave concern for human health and society. Hence, there is an urgent need to discover alternate sources of antibiotics with new structures and mechanisms. Gougerotin is a

potent broad-spectrum dipeptidyl nucleoside antibiotic that inhibits bacterial protein synthesis. It also exhibits promising anticancer, antiviral, anthelmintic, antimycoplasma, and acaricidal properties<sup>1</sup>. Moreover, it possesses a unique structure comprising a cytosine, 4-amino-4-deoxyglucuronamide, and a sarcosyl-D-serine dipeptide framework. Recently, a biosynthetic gene cluster (BGC) for gougerotin has been discovered in *Streptomyces gramineus*, and a preliminary pathway has been proposed. However, none of the enzymes have been biochemically and mechanistically investigated in-vitro. A pathway based on the studies done in *S. gramineus* has been outlined. It is proposed that GouF, annotated as cytosylglucuronic acid (CGA) synthase, first connects the nucleobase, cytosine (2), to the sugar portion of UDP-glucuronic acid 3 to form the nucleoside, CGA (4). In the next step, GouA, also known as CGA oxidase, generates 5. This is followed by transamination by putative pyridoxal phosphate (PLP)-dependent aminotransferase, GouH, to generate 4'-amino-CGA, 6. On the other hand, the modified amino acid, D-serine (10) is proposed to be obtained from cellular 3-phosphoglycerate, 7 by de novo serine biosynthesis by successive reactions catalysed by putative oxidase GouL, aminotransferase GouI, and phosphoglycerate mutase/alkaline phosphatase, GouG, respectively. On the other hand, GouN, a probable methyltransferase, is proposed to carry out the N-methylation of glycine (12), forming sarcosine (13). Thereafter, GouK, a coenzyme A-dependent protein, is proposed to create the activated amino acids, 10 and 13, which are then transferred to the amino groups of 6 and 11 sequentially by GouJ-catalysed reaction (an acyl-CoA N-acyl transferase), to generate the peptidyl-nucleoside, yunnanmycin (14). Finally, GouB, a putative amidase, is proposed to install the carboxamide in the C-6' carboxylate of 14 to form the mature antibiotic, gougerotin. In this work, we propose several in-vitro biochemical experiments to investigate the intriguing enzymatic chemistries.

## **OP-11 : Cationic Micellar Catalyzed Hydrolysis Effect on Reaction Mechanism of Mono 2-Methoxy Phenyl Phosphoramidate (MPPA) Ester**

**Ravi Prakash<sup>1</sup>, Neelesh Kumar Pandey<sup>2</sup> and R.B. Singh<sup>3</sup>**

<sup>1,2</sup>Department of Chemistry, B.S.A. College, Mathura-281004, U.P.

<sup>3</sup>Scientist 'C' (UGC), Department of Zoology, School of Life Sciences, Dr.

Bhimrao Ambedkar University, Khandari Campus, Agra-282002, U.P.

E-mail : drravichem@gmail.com, neelehpbsa1@gmail.com,

rbsinghugc@gmail.com

Reaction kinetics deals with the rate of chemical reactions and all such factors which influence the reaction rate. It further provides a satisfactory explanations for the reaction rate in terms of the possible

mechanism steps, through which the overall reaction proceeds. The most interesting aspect of the study of reaction rates is the insight it provides into the mechanism of a reaction. The dependence of reaction rates on the concentration of reactants, temperature and various other factors. Reaction of hydroxide ion with mono 2-methoxy phenyl phosphoramidate (mono ester) in presence of micellar of cationic (cetyltrimethyl ammonium bromide) detergent have been investigated at pH 8.0 to 10.0 at 40  $\pm$  0.50°C in an aqueous solution. Pseudo first order rate constant  $k$  and  $K$  have been measured spectrophotometrically by rate of appearance of inorganic phosphate during hydrolysis. The concentration of the substrate was maintained  $5.0 \times 10^{-4}$  mol dm<sup>-3</sup> for all kinetic runs (Unless otherwise specified) and that of detergents varied in between  $10^{-3}$  to  $10^{-4}$  mol dm<sup>-3</sup>. Effect of substrate concentration, pH, temperature etc.

## **OP-12 : Effect of Dimethyl Sulphide Oxidation Products on New Particle Formation in the Marine Environment**

**Janardhanan Aswathi and Deepa Janardanan\***

*Computational Chemistry & Molecular Modeling Laboratory, Department of Chemistry, School of Physical Sciences, Central University of Kerala, Kasaragod, Kerala-671325*

*\*E-mail: deepa.j@cuks.ac.in*

Dimethyl Sulphide (DMS), a primary biogenic sulphur compound emitted by marine phytoplankton, undergoes atmospheric oxidation to form Sulphuric acid (SA) and Methane sulfonic acid (MSA), which are key contributors to New Particle Formation (NPF) in the marine atmosphere<sup>1</sup>. Recent studies have revealed that SA and MSA can act synergistically to enhance particle formation in the presence of bases such as methylamines<sup>2</sup>. However, the detailed nucleation mechanism that proves this synergy and the influence of ambient atmospheric conditions remains poorly understood. Our results show that under anhydrous conditions, cluster growth proceeds through SA-MA interactions, resulting in SA-MA clusters during the outgrowth process. In contrast, increasing the relative humidity to 40% promotes the formation of mixed MSA-SA-MA clusters in the growth pathway, as water molecules facilitate additional hydrogen bonding and decrease evaporation rates, thereby making them more stable. Moreover, the calculated formation rates indicate that NPF is more sensitive to variations in SA concentration than that of MSA. We also find that the steady-state concentration of the heterodimer MSA-SA is comparable to that of SA and MSA dimers. These findings significantly advance our understanding of sulfur-driven NPF in marine environments and its impact on the atmosphere and climate.



## OP-13 : Synthesis, Biological and Molecular Docking Studies of Some Novel 1, 2, 3 Triazoles Bearing Pyrazole Moiety

Nagma Banu H.A. and Balakrishna Kalluraya\*

*Department of Chemistry, Jnanakaveri Campus, Kodagu University.  
Chikkaaluvara, Kodagu 571232, Department of Chemistry, Mangalore  
University. Mangalagangothri, Konaje 574199  
E-mail : bkalluraya@gmail.com*

Defined with dual mode of action, the hybrid molecule synthesis is an attractive strategy to endure the scientific challenges in drug discovery. In the present study, a novel class of pyrazole bearing 1,2,3-triazole by the 1,3-dipolar cycloaddition of appropriate azides with terminal alkynes carrying aryl/heteroaryl hybrid molecules are synthesized and were characterized by FT-IR, <sup>1</sup>HNMR, <sup>13</sup>CNMR, LC-MS. In-vitro Antibacterial efficacy manifests the potentiality of 1,2,3 triazole derivatives (10a-l) against gram-negative and gram-positive bacteria. Compounds 10b, 10d, 10e, 10g, 10j, 10k exhibited broad-spectrum activity with excellent and high inhibition. In the DPPH radical inhibition assay, Compounds (10e) and (10l) with standard ascorbic acid showed good radical inhibition activity at maximal inhibitory concentration. Further, the activity of 10e was validated by molecular docking study for the compound 10e showed the minimum binding energy of -11.7 kJ/mol.

## OP-14 : Sulfone Based Deep Blue Emitter for OLEDs Application

Dnyaneshwar B.K.<sup>1</sup>, Gangadhar B.<sup>1</sup> and P. Rajamalli<sup>2</sup>

<sup>1</sup>*PG Chemistry KLE's RLS institute Belagavi*

<sup>2</sup>*Material Research Center Indian institute of Science(IISC) Bangalore*

Blue organic light-emitting diodes (BOLEDs) hold a pivotal role in the field of organic electroluminescence (EL). As key components in next-generation full-colour flat-panel displays and future energy-efficient solid-state lighting, blue EL is essential for optimal performance. Nevertheless, significant challenges remain in developing highly efficient, colour-stable, and long-lasting blue-emitting materials and devices—particularly deep-blue emitters, which are crucial for achieving high-quality displays and lighting. Encouragingly, in recent years, sustained efforts by researchers have led to remarkable advancements in deep-blue OLED technologies. Hence, in this project, we synthesized sulfone-based small organic compound to obtain high performance deep blue emitters for OLEDs application. Moreover, the future perspectives and ongoing work (Initial studies) of this research frontier are also highlighted.

## **OP-15 : Interfacial Integration of Mg-Organoclay into Thin-Film Nanocomposite Membranes for Microplastic and Complex Wastewater Abatement**

**K.N. Santhosh, D.S. Aditya and S.K. Nataraj\***

*Sustainable Materials and Processes Lab, Centre for Nano & Material Sciences, JAIN University, Jain Global Campus, Bangalore- 562112*

*\*E-mail : sk.nataraj@jainuniversity.ac.in; sknata@gmail.com*

Microplastics (MPs), persistent synthetic pollutants with diverse polymeric compositions, have emerged as a pressing global concern due to their ubiquity in industrial effluents, surface waters, and domestic wastewater, and their potential ecological and human health impacts. Addressing the critical need for efficient and scalable remediation technologies, we report a novel magnesium-organoclay (MON) functionalized with amine-rich moieties to enable strong interactions with MPs via hydrogen bonding, electrostatic forces, and hydrophobic affinity. This MON was incorporated into a thin-film nanocomposite (TFN) membrane via aqueous-phase dispersion prior to interfacial polymerization with trimesoyl chloride and m-phenylenediamine, yielding a defect-free, highly hydrophilic polyamide layer. The resulting MON-TFN-0.1 membrane exhibited exceptional water permeance ( $62.39/ \text{L.m}^{-2}.\text{h}^{-1}$ ), high  $\text{MgSO}_4$  rejection (96.23%), and >96% removal of organic dyes, confirming enhanced selectivity without compromising permeability. Long-term filtration tests with Multiple industrial and sugar-processing wastewaters demonstrated excellent operational stability over 225/ h, with flux recovery ratios exceeding 98%. Significantly, the membrane achieved >97% microplastic rejection while maintaining a stable flux of  $38.28/ \text{L.m}^{-2}.\text{h}^{-1}$ . Optical microscope, Field emission scanning electron microscope (FESEM), and Differential scanning calorimetry (DSC) analyses revealed efficient MP capture and surface immobilization, attributed to robust nanoclay polyamide interactions and tailored interfacial chemistry. The integration of MON functionalized clay within the polyamide matrix not only enhances separation performance but also imparts antifouling resilience. This study establishes a scalable, multifunctional membrane platform for advanced microplastic remediation, offering a promising pathway for sustainable water treatment across diverse industrial effluent streams.

## **OP-16 : Design, Synthesis and Opto-electrochemical Properties of Novel Donor-Acceptor Based Quinoline-chalcone Derivatives as Blue-Orange Fluorescent Materials**

**Dhanashri C. Kamthe<sup>1</sup>, Sandeep R. Tapkir<sup>2</sup>, Suraj S. Mahadik<sup>2</sup> and Dinesh R. Garud<sup>1\*</sup>**

<sup>1</sup>*Department of Chemistry, Sir Parashurambhau College, Tilak Road, Sadashiv Peth, Pune-411030*

<sup>2</sup>*Department of Chemistry, University of Mumbai, Santacruz (E), Mumbai-400 098*

*E-mail : ddgarud@gmail.com*

Organic fluorescent dyes are a class of organic compounds with fluorescent properties. Their molecular structure and conjugated systems determine their specific emission colour and optical properties. Organic fluorescent molecules such as coumarins, rhodamines, boron-dipyrromethene (BODIPY), quinoline<sup>1</sup> and porphyrin derivatives display their applications in photosensitizers, organic electroluminescence, drug tracing, and even in solar cells. In this regard, the quinoline-derived chalcone<sup>2</sup> derivatives is found to be fascinating scaffold in drug discovery research.

We herein report, the synthesis of novel donor acceptor (D A) type quinoline-conjugated chalcone derivative 3 by employing Claisen-schmidt condensation reaction of quinoline-3-carboxaldehyde 1 and substituted acetophenones 2 under basic conditions. The synthesized compounds were well characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, Mass spectroscopy, electrochemical methods and X-ray analysis. Further, the electrochemical and thermal methods. Absorption and emission spectras were studied in liquid. Further, solid state emission was studied for aggregation-induced emission (AIE) effect in THF-water.

## **OP-17 : Fabrication and Evaluation of TiO<sub>2</sub>-ZnO Nanocomposites for Antimicrobial Textile Applications**

**Y.I. Shaikh<sup>1\*</sup>, G.M. Nazeruddin<sup>2</sup>, Viqar S. Shaikh<sup>2</sup> and Neeraj R. Prasad<sup>2</sup>**

<sup>1</sup>*Department of Chemistry, Abeda Inamdar Senior College, Camp, Pune-411001 Maharashtra*

<sup>2</sup>*Shivaji University, Maharashtra State, Kolhapur, 416004*

This research paper explores the synthesis, characterization, and applications of zinc oxide (TiO<sub>2</sub>-ZnO) nanomaterials, with a focus on their antimicrobial properties and potential use in textiles. The study

details the successful synthesis of  $\text{TiO}_2\text{-ZnO}$  nanoparticles using the traditional Ayurvedic method of Bhasmikaran, a process involving purification and incineration to transform zinc into a bioavailable form. The resulting nanomaterials were characterized using a range of modern analytical techniques, including DRS-UV-visible spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), Fourier transform infrared spectroscopy (FT-IR), Raman spectroscopy, photoluminescence spectroscopy, and transmission electron microscopy (TEM). The antimicrobial activity of the synthesized  $\text{TiO}_2\text{-ZnO}$  nanoparticles was evaluated, demonstrating their effectiveness against various microorganisms, which is crucial for textile applications. Furthermore, the study investigated the application of  $\text{TiO}_2\text{-ZnO}$  nanomaterials in textiles by assessing their impact on crease recovery, stiffness, and tearing strength, highlighting the potential of  $\text{TiO}_2\text{-ZnO}$  to enhance fabric performance and impart antimicrobial properties.

## **OP-18 : Synthesis of Quinoxaline Derivatives using Cobalt Doped Nano-Carbon**

**Dinesh R. Garud<sup>1\*</sup>**

*Department of Chemistry, Sir Parashurambhau College, Tilak Road, Pune 411030, (Maharashtra)*

*E-mail : ddgarud@gmail.com; dr.garud@spcollegepune.ac.in*

In recent years, N-containing heterocyclic compounds are the most valuable group of scaffolds in pharmaceuticals and bioactive natural products. In this regard, quinoxalines are a versatile class of nitrogen-containing heterocyclic compounds that shows various biological activities such as antiprotozoal, antibiotic, kinase inhibitors, anticancer, anti-inflammatory, antimalarial, antidepressant, antiviral, antihelmintic, and also active against AIDS. There are a number of synthetic strategies available for the preparation of substituted quinoxalines. The majority of protocols for synthesizing quinoxaline derivatives are linked to one or more of the limitations due to the use of expensive catalysts, need for anhydrous conditions, unsatisfactory yields, or harsh reaction conditions. Consequently, it is desirable to develop an efficient, straightforward, cost-effective, safe, and environmentally friendly method for the synthesis of quinoxalines. In continuation to our research for the synthesis of quinoxalines, we prepared Cobalt Doped Nano-carbon (FNCB-6) based solid catalyst and characterized by spectroscopic techniques like FTIR, XRD, Raman etc.

## OP-19 : Metal-Free and Site-Selective Late-Stage C–H Nitration of Heterocyclic Drug Candidates via Radical Addition Reaction

Ajay Yadav<sup>1</sup>, Neeraj Kumar Mishra<sup>1\*</sup> and In Su Kim<sup>2</sup>

<sup>1</sup>Department of Chemistry, University of Lucknow, Lucknow-226007, U.P.

<sup>2</sup>School of Pharmacy, Sungkyunkwan University, Suwon-16419, Republic of Korea

E-mail: neerajchemistry@gmail.com<sup>1</sup>; insukim@skku.edu<sup>2</sup>

A metal-free and site-selective C–H nitration approach has been developed for the late-stage modification of heterocyclic drug candidates through a radical addition mechanism. Utilizing tert-butyl nitrite as a mild and environmentally benign nitrating agent, the reaction proceeds efficiently under metal-free conditions, offering excellent regioselectivity and broad functional group tolerance. Mechanistic studies, supported by radical inhibition experiments, confirm that NO<sub>2</sub> radicals selectively attack the electron-rich aromatic region of N-heterocycles, avoiding undesired substitution on electron-deficient sites. The transformation operates under mild, scalable, and sustainable conditions, delivering nitrated products with high precision. Moreover, selective reduction of the nitro group affords aniline derivatives, highlighting the synthetic utility of this radical-mediated methodology. This work establishes a green and efficient route for the functionalization of biologically relevant N-heterocycles<sup>1</sup>, which I will explain during my poster presentation.

## OP-20 : Multicomponent and Dipolar Cycloaddition Strategies to Access Triazoles, and Pyrazoles

Sreelekha K.M.<sup>1</sup> and Beneesh P.B.<sup>2\*</sup>

<sup>1</sup>Department of Chemistry, Mangalore Institute of Technology & Engineering, Moodabidri, 574225, Mangalore

<sup>2</sup>Department of Chemistry, National Institute of Technology Karnataka, Surathkal, 575 025, Mangalore

E-mail : pbbeneesh@nitk.edu.in

An efficient [3+2] annulation reaction between aldehyde hydrazones and in situ-generated propionaldehyde, affording pyrazole-4-carboxaldehyde under mild reaction conditions, is reported. The reaction first involves propionaldehyde formation from propargyl-p-toluenesulfonate via a base-free Kornblum oxidation in DMSO, followed by annulation with hydrazone. Interestingly, the pyrazole-4-carboxaldehyde further endured a unique cascade reaction with hydrazine and propargyl tosylate in one-pot, yielding synthetically challenging bipyrazole carboxaldehydes in moderate yields.

Also, an investigation for synthesizing hybrid molecular scaffolds in which a benzyl bridge links various 1,3-diones and 1,2,4-triazoles

has been established using aldehyde hydrazones through multicomponent reaction. This three-component, one-pot reaction was accomplished by first treating 4-hydroxycoumarin, trans- $\beta$ -nitrostyrene, and aldehyde hydrazone in the presence of sodium carbonate. Further, this protocol was successfully expanded to other 1,3-diones, such as dimedone and 4-hydroxy-2-quinolone.

### **OP-21 : Targeting Antiproliferation and Antioxidant Properties of 3-Substituted 2-Aminopyrimidine Derivatives**

**Rajendra Nimbale, Siraj B. Shaikh, Pranav Tambe, Vishal Sathe, Hanumant Dupade and Khursheed Ahmed\***

*M.C.E. Society's Abeda Inamdar Senior College, Advanced Scientific Research Laboratory, Azam Campus, Camp, Pune-01, MH*

3-substituted 2-aminopyrimidine derivatives were prepared from 2-amino pyrimidine as starting material. The prepared compounds differ from each other by the substitutions of their 3-substituted their phenyl ring and group. The 2-aminopyrimidine derivative were tested for their anti-proliferative action against MCF-7 cell and antioxidant activity. Some of the compounds exhibited quite good anti-proliferative activity, and others showed excellent antioxidant activity. These activities were shown to be impacted by the structural changes.

### **OP-22 : Theoretical Exploration of Two-Dimensional Materials for Optical, Thermal and Electrical Properties**

**Dhananjay and Ravi Kumar Kanaparthi\***

*Department of Chemistry, Central University of Kerala, Tejaswini hills, Periyar, Kasaragod, Kerala, 671316*  
*E-mail : dhananjay.2301107005@cukerala.ac.in; rkchem@cukerala.ac.in*

Two-dimensional materials have emerged as the new hotspot for current research interests in material sciences. Since the revelation of graphene in 2004, the scientific community has delved into two-dimensional materials research in the hunt of better and more efficient sensors, photochemical devices, optoelectronic devices and thermoelectric devices. Janus Materials are a kind of 2D material that has been exploited more over its symmetric counterparts because of their out of plane symmetrical characteristics and hinting towards intra piezoelectric effects as well. The current work ongoing on the Janus monolayer TiSeS has been carried out using Density Functional Theory as implemented in Quantum ESPRESSO 7 with GGA-PBE XC functional. GGA-PBE was used as per the suggestion of literature and has been proved to be an excellent functional for carrying out several

janus monolayers. The structural optimization of the monolayer yielded the lattice constant to be 3.47 Å corresponding with the literature. The band structure was calculated further to understand the electronic property of the monolayer and it was found to be a semiconductor with a little bandgap. Upon further calculations, the optical properties of monolayer were calculated and the real and imaginary part of the dielectric constant was produced. These 2-D materials are the present pinnacle of innovation and will just thrive higher over time. The theoretical exploration of these materials and the computational simulations are a necessary and crucial step to bring in some extra time and cost cuttings.

### **OP-23 : Pyrazine-1,3,4-Oxadiazole Hybrids as Inhibitors of Thymidylate Synthase: Synthesis, Characterization, and Molecular Docking**

**Amin Shaikha, Ashpak Shaikh and Khursheed Ahmed\***

*Department of Chemistry, Abeda Inamdar Senior College, Advanced Scientific Research Laboratory, Azam Campus, Camp, Pune-01*

This study investigates the synthesis, characterization, and molecular docking of pyrazine-1,3,4-oxadiazole hybrid compounds as inhibitors of thymidylate synthase (TS). The hybrids were synthesized and characterized using HRMS, FTIR, and NMR spectroscopy. Molecular docking studies revealed the binding interactions of the compounds with the TS active site, suggesting their potential as effective inhibitors. ADMET analysis was performed to assess the drug-like properties of the hybrids, indicating favourable profiles for absorption, distribution, metabolism, excretion, and toxicity. These results highlight the potential of pyrazine-1,3,4-oxadiazole hybrids as promising candidates for the development of TS inhibitors.

### **OP-24 : Synthesis, Spectral, Electrochemical Properties and Biological Study of Substituted Pyrimidine with Acetyl Pyrazine Chalcone and Urea**

**Ataur Rehman Shaikh<sup>1,2</sup>, Heena A. Khan, Parnov Tambe and Khursheed Ahmed<sup>1,2\*</sup>**

<sup>1</sup>*Department of Chemistry and Post Graduate Research Centre, Abeda Inamdar Senior College, Pune-411001, Maharashtra*

<sup>2</sup>*Advanced Scientific Research Laboratory, Abeda Inamdar Senior College, Pune-411001, Maharashtra*

New five new substituted pyrimidine were synthesised by using pyrazine chalcone derivatives with Urea. All compounds were characterised by Mass, <sup>1</sup>H NMR, and IR spectroscopy. Such compounds have shown their application as anti-microbial, anti-fungal, anticancer.



Antioxidant activity of several representative compounds was explored in DPPH (2,2-diphenyl-1-picrylhydrazyl) assay, revealing significant scavenging for substituted derivatives endowed with pyrazine analogues antioxidant was shown by the representative compounds tested. All compounds were submitted for evaluation of their antifungal and antibacterial activity.

### **OP-25 : Synthesis, Spectroscopic Analysis, and Structural Characterization of Thiazole Chalcone Compounds**

**Shaikh Faruk Shabbir<sup>1,2</sup>, Ataur Rehman Shaikh<sup>1,2</sup> and Doke Kailas\***

<sup>1</sup>*Department of Chemistry and Post Graduate Research Centre, Abeda Inamdar Senior, College, Pune-411001, Maharashtra*

<sup>2</sup>*Advanced Scientific Research Laboratory, Abeda Inamdar Senior College, Pune-411001, Maharashtra*

The synthesis and characterization of chalcone derivatives of thiazole are of significant interest due to their potential applications in medicinal chemistry, pharmaceutical science. This study reports a systematic approach to the synthesis of chalcone derivatives of Thiazole, involving the condensation of aromatic aldehyde with thiazole precursors under optimized conditions to achieve high yields and purity. The synthesized compounds were characterized using various spectroscopic techniques, including <sup>1</sup>HNMR, IR, and UV-Vis spectroscopy technique, the resulting chalcone derivatives of thiazole is subjected for bioactivity like anti-microbial, antifungal antibacterial etc activity. We are synthesised five deferent types of Chalcone and study the biological activity.

### **OP-26 : Detection of Fingerprint Residues at Crime Scenes Using FTIR and Raman Spectroscopy: Analysis of External Residues**

**Chitrakara Hegde<sup>1,2\*</sup>, Sheethal<sup>1</sup> and Ann Mariya Joseph<sup>1</sup>**

<sup>1</sup>*Department of Chemistry, Alliance University, Bengaluru- 562106*

<sup>2</sup>*CoE in Water Research, Alliance University, Bengaluru- 562106*

\*E-mail : chitrakarahegde@gmail.com

Fingerprint residues found at crime scenes encompass a complex mixture of endogenous secretions and exogenous environmental contaminants. This study presents the combined application of Fourier Transform Infrared Spectroscopy (FTIR) and Raman Spectroscopy to detect and thoroughly characterize these fingerprint residues. FTIR provides detailed chemical profiling by identifying organic and inorganic components, including lipids, amino acids, and pollutants. Raman spectroscopy complements this by offering molecular fingerprinting

with high spatial resolution, enabling the identification of trace contaminants such as dirt, grease, cosmetics, inks, and explosive residues without destructive sample preparation. Together, these vibrational spectroscopic techniques deliver a comprehensive, non-invasive chemical and molecular analysis of fingerprint residues. This integrated approach enhances forensic investigations by linking individuals to crime scenes through detailed residue composition, while also offering contextual clues about suspect activities and environmental exposure. The use of FTIR combined with Raman spectroscopy represents a powerful toolset for advancing forensic fingerprint analysis in criminal investigations.

## **OP-27 : Enhanced Protein Separation using Ag-ZnO Integrated Polyphenylsulfone Ultrafiltration Membranes**

**Panchami H.R.<sup>1,2</sup> and Arun M. Isloor<sup>2</sup>**

<sup>1</sup>*Department of Chemistry and Biochemistry, M. S. Ramaiah College of Arts, Science and Commerce, MSR Nagar, MSRIT post, Bengaluru 560054*

<sup>2</sup>*Membrane and Separation Technology Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, Mangalore 575025*

<sup>\*</sup>*E-mail : isloor@yahoo.com*

In this study, polyphenylsulfone (PPSU) nanocomposite membranes incorporated with silver-doped zinc oxide (Ag-ZnO) nanoparticles were fabricated using the dry/wet phase inversion technique. Spectroscopic and microscopic analyses confirmed the successful synthesis of Ag-ZnO nanoparticles and their uniform distribution within the PPSU matrix. Incorporation of 1.5 wt.% Ag-ZnO significantly improved membrane morphology, surface hydrophilicity, and surface charge, leading to enhanced pure water permeability, antifouling performance, and protein rejection. The optimized membrane (AZM-2) exhibited a high pure water permeability of 196.95 L m<sup>-2</sup> h<sup>-1</sup> bar<sup>-1</sup>, a flux recovery ratio of 68.2%, and a molecular weight cut-off of 7196.3 Da. Protein rejection values for BSA, egg albumin, and pepsin reached 92.1%, 86.8%, and 73.4%, respectively. These results demonstrate that Ag-ZnO-modified PPSU membranes possess superior hydrophilic and functional properties, making them promising candidates for efficient protein-rich wastewater treatment applications.

## **OP-28 : Preparation and Characterization of Breathable Nano Biopolymer layer for Protective Medical Mask**

**Vishwanath T.\* and Sayana K.V.**

*Department of Materials Science, Mangalore University, Mangalagangothri-574199*  
*E-mail : vishutcg@gmail.com*

A large amount of synthetic single-use medical masks are produced

every year, resulting in increased biowaste production and biohazardousness. Sustainable medical devices play an important role in environmental protection due to minimal waste production and waste management. In this study, a PVA-chitosan nano-layer was fabricated as a protective layer for medical masks using electrospinning technology to filter bacteria and viruses. The material was characterised by FTIR, XRD, FE-SEM, and contact angle measurements. The mechanical properties of the nano layer were improved by adding the bio-synthesised nano-titania particles. The water absorption capacity and solubility of the composite nanofiber layer were evaluated. The mask model exhibited excellent splash resistance to the artificial blood and microbial cleanliness performance. The breathability of the mask was optimised along with the bacterial and viral filtration efficiencies. The composite nanofiber mesh confirmed the film's biodegradability, with visible structural disintegration and weight loss. The developed mask model demonstrated a promising integration of biopolymer-based electrospun nanofibers and herbal phytochemicals, offering a sustainable alternative to synthetic medical masks.

### **OP-CYSA-01 : Synthesis and Characterisation of Some Biopolymers**

**Arati. J. Prajapati<sup>1,2</sup>, Meeta V. Patel<sup>2</sup>, H.D. Chaudhari<sup>2</sup> and J.J. Vora<sup>1</sup>**

<sup>1</sup>Adarsh Science (P.G.) Collage, Patan

<sup>2</sup>Department of Chemistry, Patan, Hemchandracharya North Gujarat University, Patan-384265

E-mail : Prajapatiarti09071999@gmail.com

This study highlights the chemical modification of natural biopolymers to enhance their functional properties and broaden their potential applications. Starch, a safe, biodegradable, and easily available biopolymer, was selected as the base material. Through chemical modification, new functional groups were introduced into the starch structure, aiming to improve its physical, chemical, and surface properties. The modified starch was carefully characterized using different methods to analyse changes in molecular structure, particle size, morphology, and surface nature. Results clearly indicated that the modification process was successful, showing noticeable differences when compared to native starch. These changes suggest improved stability, solubility, and functionality. Such modified biopolymers hold great promise for use in medicine, pharmaceuticals, food, packaging, and other industrial applications. Keywords: Biopolymer modification, starch, characterization

## **OP-CYSA-02 : Tailoring Polysulfone Mixed Matrix Membranes: Bridging Polymer Science and Nanotechnology for Sustainable Water**

**Deepthi P.V.<sup>1,2</sup> and Vijesh A. M.<sup>2,3\*</sup>**

<sup>1</sup>*Department of Chemistry, Nehru Arts and Science College, Kanhangad, Kannur University, Kerala-671314*

<sup>2</sup>*P.G. and Research Department of Chemistry, Government College, Kasaragod, Kannur University, Kerala-671123*

<sup>3</sup>*P.G. Department of Chemistry, Payyanur College, Payyanur, Kannur University, Kerala-670327*

<sup>\*</sup>*E-mail : vijeshnambisan@gmail.com*

The rapid population growth has driven industrial expansion, particularly in textiles, leading to the release of toxic wastewater that harms the environment and human health. The wastewater must be properly treated before releasing it into the environment. Membrane technology is widely used for water treatment, and nanotechnology helps improve its performance. Hollow fiber membranes are a great option for water treatment since they have a higher surface area per volume than flat sheet membranes.

An outline of polysulfone composite membranes with nano additives is provided in this abstract, emphasizing their characteristics and possible uses in dye rejection research. Distinct nanocomposite membranes with improved structural and functional characteristics were fabricated by the phase inversion approach. In-depth characterisation methods shed light on the chemical and morphological characteristics. Experiments were conducted using SEM, AFM, water absorption, contact angle, water permeability, antifouling properties, and dye rejection. The new membrane's ability to remove the dyes RO16 and RO5 was improved by the use of nano additions. According to the results, the compounds have a lot of potential to enhance membrane characteristics without compromising their rejection capacities. This paper will explain the findings of such investigations.

## **OP-CYSA-03 : Design, Synthesis and Biological Evaluation Of (5-Substituted 2-Phenyl-1h-indol-3-yl)-n-(Pyridin-4-yl)Methanimine and Its Derivaties**

**Pooja Pasodi, Vijaykumar T. Katkar and Anand R. Saundane\***

*Department of Studies and Research in Chemistry, Gulbarga University, Kalaburagi-585 106, Karnataka*

*E-mail : arsaundane@rediff.com*

Heterocyclic compounds acquiring more importance in recent years because of their broad pharmacological activities. Nitrogen containing five and six member heterocyclic compounds have occupied enormous

significance in the field of medicinal chemistry. Hence, it is not surprising that indoles act as lead compounds and are key building blocks in numerous pharmaceuticals. From ancient time, indole derivatives constitute an important class of therapeutic agents in medicinal chemistry including antihypertensive, anti-proliferative, antiviral, antitumor, analgesic, anti-inflammatory, antioxidant, antimicrobial, anticancer etc.

The precursor N-((5-substituted 2-phenyl-1H-indol-3-yl)methylene)pyridin-4-amines (3a-c) were prepared by 5-substituted 2-phenyl-1H-indole-3-carbaldehydes (1a-c) with pyridin-4-amine (2). Compounds (3a-c) underwent cyclocondensation reaction with thioglycolic acid, Phenyl acetyl chloride and Acetyl chloride at refluxed temperature afforded 2-(5-substituted 2-phenyl-1H-indol-3-yl)-3-(pyridin-4-yl)thiazolidin-4-ones (4a-c). 3-phenyl-4-(5-substituted 2-phenyl-1H-indol-3-yl)-1-(pyridin-4-yl)azetidin-2-ones (5a-c) and 4-(5-substituted 2-phenyl-1H-indol-3-yl)-1-(pyridin-4-yl)azetidin-2-ones (6a-c), respectively. The structures of newly synthesized compounds were characterized by their spectral studies and elemental analysis. These compounds were screened for their antimicrobial and antioxidant activities. The compounds 5b showed potent RSA and Compound 4b and 6b exhibited potent/equipotent antimicrobial activities.

## **OP-CYSA-04 : Novel ionic Poly(VBC-co-VI) Nanoparticles for the Fabrication of Thin Film Nanocomposite Membranes for Dye and Salt Rejection**

**Nidhi Regina Mendonca and Arun M. Isloor**

*Membranes and Separation Technology Lab, Department of Chemistry,  
National Institute of Technology Karnataka, Surathkal-575025  
E-mail : isloor@yahoo.com@yahoo.com*

Water is essential for the survival of all living forms on Earth. However, this natural resource is depleting as a result of human activities. This work examines a potential method for salt containing dye wastewater treatment by using thin film composite (TFC) membranes. These membranes were created through the interfacial polymerization technique on a 15 wt% polysulfone macroporous support. The dense polyamide layer resulting from the interfacial polymerization reaction was incorporated with novel ionic poly(VBC-co-VI) nanoparticles synthesized via quaternary precipitation polymerization reaction of the monomers 1-Vinyl imidazole (VI) and 4-Vinylbenzyl chloride (VBC) in the presence of the free radical initiator 2,2'-Azobis(2-methylpropionitrile) (AIBN) with acetonitrile as the solvent in a single step. The addition of the nanoparticles into the PA layer

enhanced the water permeability and the rejection performance of the membranes. The fabricated thin film nanocomposite membranes demonstrated an improved dye rejection rate of 98% for Reactive Black 5 and over 95% for Sunset Yellow FCF, both possessing a 100 ppm concentration. The rejection of salts NaCl, MgCl<sub>2</sub>, Na<sub>2</sub>SO<sub>4</sub>, and MgSO<sub>4</sub> at a concentration of 1000 ppm, was also carried out with the rejection rates being 36% for NaCl, over 50% for MgCl<sub>2</sub>, 85% for Na<sub>2</sub>SO<sub>4</sub>, and 85% for MgSO<sub>4</sub>.

### **OP-CYSA-05 : High-Performance NH<sub>2</sub>-UiO-66@PSF Membranes for the Selective Removal of Pb(II) and Cd(II) from Water**

**Shivarama B.<sup>1</sup> and Arun M. Isloora**

*<sup>1</sup>Membrane and Separation Technology Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, Mangalore-575 025*

The accelerating pace of urbanization and industrialization has intensified global concerns over the availability of clean water, breathable air, and renewable sources of energy. In this work, hybrid membranes incorporating NH<sub>2</sub> UiO 66 metal–organic frameworks (MOFs) were fabricated and evaluated for their efficiency in removing lead and cadmium ions from aqueous solutions. NH<sub>2</sub> UiO 66 was synthesized in the laboratory following a slightly modified version of a previously established procedure. The resulting MOF was thoroughly characterized through scanning electron microscopy (SEM), thermogravimetric analysis (TGA), Brunauer–Emmett–Teller (BET) surface area measurement, Fourier transform infrared spectroscopy (FTIR), and X ray diffraction (XRD). The material showed excellent water stability. To fabricate the hybrid membranes, the MOF was incorporated at varying loadings of 0.5 wt%, 1.0 wt%, and 3.0 wt% into a polymeric matrix. The resulting membranes were tested for their heavy metal removal efficiency. Among them, the M 1 membrane containing 0.5 wt% of MOF exhibited the highest pure water flux. Water uptake and porosity analysis confirmed the hydrophilic nature of the prepared membranes. Furthermore, irreversible fouling was reduced by about 49.77% and total fouling by approximately 24.38% with the inclusion of 0.5 wt% MOF compared to the pristine sample. Heavy metal rejection experiments performed at 500 ppm feed concentration and 2 bar pressure. M 1 membrane containing 0.5 wt% of MOF demonstrated 55.54% rejection for lead and 74.94% rejection of cadmium. These findings highlight the promise of NH<sub>2</sub> UiO 66–based hybrid membranes for the effective removal of toxic heavy metals from water.



## OP-CYSA-06 : First Regioselective Iodocyclization Reaction of 3-aryl-5-(allenylthio)-4H-1,2,4-triazoles

Snehal S. Kondhalkar, Kamlesh A. Nerkar and Dinesh R. Garud\*

Department of Chemistry, Sir Parashurambhau College, Tilak Road, Pune 411030, (Maharashtra)

E-mail : ddgarud@gmail.com; dr.garud@spcollegepune.ac.in

In recent decades, 1,2,4-triazoles and their fused heterocyclic derivatives exhibits interesting biological activities. Systems consisting of nitrogen and sulphur atoms in the same heterocycle shown outstanding properties and are useful in the creation of pharmaceutically important substances and functional organic materials. On the other hand, iodocyclization of an unsaturated C–C bond with a wide variety of nucleophiles, including N-, O-, S-, and Se-nucleophiles become powerful tool for the synthesis of various heterocycles.

In line with our ongoing efforts to develop efficient methodologies for investigating a new class of heterocyclic compounds that may possess potential biological activities, herein for the first time, we describe the regioselective iodocyclization reaction of 3-aryl-5-(allenylthio)-4H-1,2,4-triazoles **2** in which 1,2,4-triazolyl nitrogen acts as an internal nucleophile on allenyl-carbon to provide fused heterocyclic derivatives 6-iodo-2-aryl-7H-[1,2,4]-triazolo[5,1-b][1,3]thiazines **3**. The structure of synthesized 6-iodo-2-aryl-7H-[1,2,4]-triazolo[5,1-b][1,3]thiazines **3** was confirmed by the <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and mass spectroscopic analysis. Further extension of current strategies is under progress in our group.

## OP-CYSA-07 : Sustainable Waste Water Purification via Integration of novel COF@UiO-66 Dual-Layer PVDF/PEI Hollow Fiber Membranes

Nethravathi Prabhakar<sup>1</sup>, Arun M. Isloor<sup>1\*</sup>,

Mohd Hafiz Dzarfan Othman<sup>2</sup> and Ahmad Fauzi Ismail<sup>2</sup>

<sup>1</sup>Membrane and Separation Technology Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, Mangalore, Karnataka-575025

<sup>2</sup>Advanced Membrane Technology Research Center (AMTEC), Universiti Teknologi Malaysia, Skudai, Johor Bahru 81310, Malaysia

\*E-mail : isloor@yahoo.com

Water is the vital component that plays decisive role in sustaining life forms on the planet. Several hazardous contaminants like dyes and heavy metal ions are ruining the natural essence of water. In this work, metal organic framework UiO-66 grafted with cost-effective covalent organic framework was used as an additive in the fabrication of dual layer hollow fiber membranes. The polymers used for the



membrane fabrication are polyether imide and polyvinylidene fluoride. The as synthesized MOF and COF@UiO-66 were intensively characterized for the successful grafting. The resulting membranes were also characterized for their morphology, porosity, thermal and mechanical stability via FESEM, molecular weight cutoff, TGA, and UTM analysis respectively. The performance of the membranes was optimized for different loadings of the additive and with different outer flow dope rates, for the removal of heavy metal ions and dyes. The optimized composition having 1.0 wt. % of the functionalized MOF exhibited a pure water permeability of  $117.5 \text{ Lm}^{-2}\text{h}^{-1}\text{bar}^{-1}$  with rejections percentages of >99.99% and 69.58% for lead and mercury along with >99% and >98% rejection for congo red and reactive black dyes. The membranes also exhibited good antifouling behaviour with a fouling rejection ratio of 74%.

## PHYSICAL CHEMISTRY SECTION

### Sectional President's Address

#### **Molecular-Level Insights into Sorption and Extraction: Role of Ionic Liquids and Deep Eutectic Solvents in Enhancing Physicochemical Processes**

**Ramesh L. Gardas**

*Department of Chemistry, Indian Institute of Technology Madras,  
Chennai 600 036*

*E-mail: gardas@iitm.ac.in*

The development of efficient and sustainable separation processes is increasingly vital in addressing challenges such as water pollution and critical metal recovery from electronic waste. Ionic liquids (ILs) and deep eutectic solvents (DESs) have emerged as promising functional fluids due to their unique physicochemical properties - such as tunable polarity, low volatility, and structural versatility.

This talk will explore the mechanistic role of ILs and DESs as performance-enhancing additives in sorption and extraction processes. Special emphasis will be placed on how intermolecular interactions - such as hydrogen bonding,  $\pi$ - $\pi$  stacking, and electrostatic effects— govern solute-solvent affinities and influence separation efficiency. The integration of computational methods, including density functional theory (DFT) and COSMO-RS, provides a deeper understanding of solvation thermodynamics, selectivity trends, and molecular recognition in complex aqueous environments.

Physical chemistry aspects such as solvation dynamics, thermophysical properties, and phase behaviour will be discussed in the context of removing micropollutants from wastewater and recovering strategic metals (e.g., lithium, cobalt) from spent lithium-ion batteries. The reusability and physicochemical stability of ILs and DESs will also be analyzed, underscoring their potential for scalable and environmentally benign applications.

By combining molecular-level modeling with macroscopic process insights, this work highlights how physical chemistry can drive innovation in green separation technologies.

## **PIL-01: Thermally Stable Ionic Nanoreactors for Facile Synthesis of Advanced Materials under Ambient Conditions**

**Arvind Kumar**

*Salt and Marine Chemicals Division  
CSIR-Central Salt and Marine Chemicals Research Institute G. B. Marg,  
Bhavnagar-364002, Gujarat  
E-mail: arvind@csmcri.res.in*

Room temperature ionic liquids (RTILs) are the organic analogues of inorganic molten salts with melting temperature <100°C. Being ionic in nature, these compounds are versatile in terms of solvent properties such as low volatility, high thermal stability, wide liquid range and good solvating ability. In view of flexibility of choice of cations or anions, RTILs can be designed as low viscosity media suitable for self-assembling of amphiphile molecules or also can be designed as surfactants by incorporating amphiphilic character in either cation or anion or in both the constituents. Therefore, with extraordinary properties it has been possible to include RTILs as media or as a surfactant or both for construction of colloidal formulations/self-assembled structures. We have constructed thermally stable ionic nanoreactors by judicious choice of ionic liquid-based surfactants and ionic liquid/deep eutectic-based solvent as polar or non-polar components. These ionic nanoreactors have been used for preparation of shape/size-controlled nanomaterials/quantum dots, metal organic frame works (MOFs) suitable for advanced applications. The presentation mainly focuses on design, development, characterization and utilization of some specific systems for synthesis of advanced materials under ambient conditions.

## **PIL-02: Physicochemical and Thermodynamic Evaluation of Cationic and Anionic Dye-Surfactant Interaction and its use in Photogalvanic Cell for Solar Energy Conversion**

**Prem Prakash Solanki**

*Department of Chemistry, Institute of Science, Banaras Hindu University,  
Varanasi-221005, Uttar Pradesh  
E-mail: ppsolanki@bhu.ac.in, ckmallbhu23@gmail.com*

The dye-surfactant interaction has crucial role in solubilization and stabilization of dyes, which directly influences the performance of photogalvanic (PG) cell. Here, Nile Blue A (NB-A, +) and Acid Blue 25 (AB-25, 6), with SDS, CTAB, and tween 80 surfactants using spectrophotometric and conductometric techniques were investigated. The stability of dye-surfactant complex formation was verified on the

basis of thermodynamic parameters. NB-A showed significant bathochromic shifts with SDS and CTAB, while negligible spectral changes with tween 80. In contrast, AB-25 was displayed pronounced spectral peak shifts with CTAB and tween 80, but only minor changed with SDS. Conductometric studies revealed that the CMC of SDS decreased with of NB-A ( $8.21 \rightarrow 7.35$ , mM) but increased with AB-25 ( $8.21 \rightarrow 9.0$ , mM). Similarly, CMC was slightly inhibited by NB-A ( $0.9 \rightarrow 1.0$ , mM), whereas AB-25 promoted micelle formation, NB-A and AB-25 showing distinct blue and red shifts in its absorption peaks with CTAB, respectively. Tween 80 showed negligible interaction with NB-A but notable shifts with AB-25, suggesting stronger hydrophobic incorporation of AB-25 into the micellar core. Thermodynamic parameters (degree of ionization, counter-ion binding, Gibbs free energy of micellization, partition coefficient, and free energy of partitioning) confirms that micellization is spontaneous in all systems but more strongly favored in NB-A–SDS and AB-25–CTAB/Tween 80 combinations. The interaction strength follows the order as: SDS–NB-A > CTAB–NB-A > Tween 80–NB-A, and AB-25. Thus, the dye (NB A) and surfactant (SDS) having opposite charges must have a very strong interaction and would be also give a significant result of electrical parameters in PG cell. Therefore, before going to photogalvanic study for solar power conversion, the present type studied must be helpful to find out an efficient dye-surfactant complex which would enhance the performance of PG cell for its sustainable development in future.

### **PIL-03: Thermophysical Properties of Industrial Solvents and their Greener Alternatives**

**Ranjan Dey**

*Thermophysical Properties Lab, Department of Chemistry, Birla Institute of Technology and Science, Sancoale, Goa, 403726*  
*E-mail: ranjandey@goa.bits-pilani.ac.in*

Thermophysical properties of liquid mixtures play a significant role in determining their applications in multifarious fields like pharmaceuticals, solvent extraction and recovery, heat and mass transfer processes, etc. The thermophysical properties of binary and higher order liquid mixtures of widely used industrial solvents such as dimethyl sulfoxide (DMSO), N-methyl-2-pyrrolidone (NMP), N, N-dimethylacetamide (DMAc), etc. gives us an understanding of their physico-chemical nature, structural changes occurring on mixing the constituent components and the molecular interactions occurring in these mixtures. Experimental determination of density( $\rho$ ), ultrasonic velocity( $u$ ), viscosity( $\eta$ ), refractive index ( $n_D$ ) has been carried out on the aforementioned systems at varying temperatures. Estimation of excess molar volumes ( $V_m^E$ ), coefficient of thermal expansion ( $\alpha_P$ ),

adiabatic compressibility ( $\beta_S$ ) and their excess counterparts from the experimental data gives us an insight about the deviations of these mixtures from ideal behavior. Most of the industrial solvents are hazardous for the environment since they are released as volatile organic compounds in the atmosphere which are carcinogenic, mutagenic and adversely affect human health and aquatic life. Sustainable and greener solvent systems such as Deep Eutectic Solvents (DESs) will be tested to envisage their role as alternatives to these hazardous VOC solvents.

#### **PIL-04: Functional Nanomaterials for Sustainable Developments**

**Harish Kumar**

*Department of Chemistry, School of Basic Sciences, Central University of Haryana, Mahendergarh-123029  
E-mail: harishkumar@cuh.ac.in*

Nanomaterials find use in energy storage devices, sensors, corrosion inhibitors, antibacterial agents, and the removal of environmental pollutants. Advanced nanostructured materials can be customized for different industrial applications. The production of metal nanoparticles/conducting polymers-based nanomaterials for multifunctional applications according to the demand of the industry is a challenging task. These nanomaterials of the future could revolutionize materials of the 21<sup>st</sup> century.

#### **PIL-05: Studies of Ultrasonic of KBr in Dioxan and Water Solvent Mixture at 303.15K**

**Ravi Prakash<sup>1</sup>, Ritu Rani Chaudhary<sup>2</sup>, and R.B Singh<sup>3</sup>**

*<sup>1,2</sup>Department of Chemistry, B.S.A. College, Mathura-281004, U.P.*

*<sup>3</sup>Scientist 'C' (UGC), Department of Zoology, School of Life Sciences, Dr.*

*Bhimrao Ambedkar University, Khandari Campus, Agra-282002, U.P.*

*E-mail: drravichem@gmail.com, ritumjp@gmail.com, rbsinghuge@gmail.com*

The dissolution of electrolyte in various solvents is responsible for structure maker or structure breaker. Viscosity and density data leads an insight to the state of association of the solute and the extent of interaction of the solute with the solvent. The present work mainly deals with the reflects the ion-ion, ion-solvent and solvent-solvent interaction KBr solution in 10%,20% and 30% in dioxan and water mixture Various acoustic parameters like isentropic compressibility ( $B_s$ ) intermolecular free length ( $L_f$ ), apparent molar volume ( $\phi_k$ ), molar sound velocity ( $R$ ), acoustic impedance ( $Z$ ) of KBr in 10%, 20%, 30% and dioxan and water solvent mixture at 303.15K have been determined from ultrasonic velocity ( $V$ ), density ( $\rho$ ) and relative viscosity ( $\eta_r$ ) of the solution. These parameters are related with the molar

concentration of the solution and reflects the distortion of the structure of the solvent in dioxan and water mixture when the solute is added to it.

## **PIL-06: Sustainable Preparation of Photo-Catalytically Active Nanomaterials and Their Composites with 2D Materials using Ionic Liquids**

**Tejwant Singh Kang**

*Department of Chemistry, UGC Sponsored Centre for Advanced Studies-II,  
Guru Nanak Dev University, Amritsar 143005  
E-mail: tejwtwantsinghkang@gmail.com*

Ionic liquids (ILs) and specifically surface-active ionic liquids (SAILs) cater to the needs for shape and size control as proficient templating agents in the synthesis of different nanomaterials. ILs offer structure directing effects via inherent bi-continuous structures formed by the segregation of polar and nonpolar domains. However, on the contrary, SAILs, owing to their surface activity, self-assembling nature and interactions with the ionic head groups, offer great deal of templating effect in the nucleation and growth of nanoparticles. Task specific metal-based ILs (MILs) or binary mixtures of ILs with other greener solvents act multifunctionally as metal ions precursors as well as the stabilizing agents, assisting in the preparation of a variety of nanomaterials. SAIL-templated synthesis of noble metal based nanoparticles has paved a way for a new sustainable and facile methodology for the shape and size control. Due to their ability to lower the surface tension of water and intercalate between the 2D bulk materials, introduction of SAILs in exfoliating 2D nanomaterials and in-situ conjugating these with other NPs develops a whole new variety of nanocomposites showing combined properties of the heterojunction formed between the 2D nanomaterial and the noble metal NPs.<sup>7</sup> The utilization of diverse area of nanomaterials in different photocatalytic applications is a progressing and recent area of research. We have utilized distinctive facile methods of preparation of NPs, their composites with 2D nanomaterials, involving the templating effect of SAILs, and their utilization in photocatalytic water remediation and water splitting applications.

## **PIL-07: Thermodynamics in Universe and Day to Day Life**

**Kalpna Kumari**

*Department of chemistry, Dr. L. K. V. D. College Tajpur, L N M U Darbhanga  
E-mail: Kalpna.chemistry@rediffmail.com*

Thermodynamics - a discipline of the physical science that define

heat, work and transformation of energy. Physical system in energy perspective best described by thermodynamics. It is more important in relation to the understanding of thermal system in industry, as well as supporting energetic process in living organisms and interaction of matter and energy. Present paper defines how matter and energy interact to describe different law of thermodynamics which can be applied in day-to-day life. It also defines the existence of universe and future of universe.

Fluidity, superconductivity and quantum computing system, financial modelling and AI can be improved with the help of Quantum thermodynamics.

Thermodynamics in context of universe - thermodynamics describes the universe is a vast isolated, irreversible system with constant mass-energy. As first law of thermodynamics describes law of conservation of energy better describes in everyday life as meditation when we meditate, our body started heating and release energy in the form of waves of specific frequency which connect the frequency of same type of wave in the universe and we get blessing and acquire power, which may be the wave of positive force and negative force conserved in the universe depends up on which type of wave you released.

The second law states that total entropy of the universe (a measure of disorder) always increases overtime. The universe started from a hot dense state and has been expanding and cooling leading to process like star formation and the eventual dispersion of energy in to a state of maximum entropy known as heat death.

Thermodynamics in day-to-day life -The preparation and subsequent cooling of a cup of coffee are governed by the second law of thermodynamics, photosynthesis, metabolism, cooking of food many more example of thermodynamics.

## **PIL-08: Development of Sustainable Heterogeneous Catalysts for Energy and Environmental Applications**

**Venkata Krishnan**

*School of Chemical Sciences, Indian Institute of Technology Mandi,  
Himachal Pradesh.  
E-mail : vkn@iitmandi.ac.in*

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. Our research group has recently developed several two-dimensional materials supported on nanostructured photocatalysts 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, our group has also utilized these materials for plastics upcycling, carbon dioxide conversion and Green organic transformations, either by functionalization or doping with a heteroatom. The highlights of the ongoing research work of our group in sustainable chemistry and heterogeneous catalysis will be presented.

### **PO-CYSA-01: Revealing Thermo-responsive Lyotropic Mesophases and Microheterogeneity in a Protic Ionic Liquid**

**Bignya Rani Dash, Ashok Kumar Mishra\* and Ramesh L. Gardas\***

*Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036  
E-mail: mishra@iitm.ac.in, gardas@iitm.ac.in*

Ionic liquid crystals (ILCs), which bridge the ordered structure of crystalline solids and the fluidity of isotropic liquids, have emerged as transformative materials for energy and optoelectronic technologies. Their modular ionic structures, tunable conductivity, anisotropic organization, and thermal stability have enabled diverse applications in energy storage, optoelectronics, sensing, catalysis, and responsive materials. A key feature that governs their macroscopic behavior is nanoscale heterogeneity, arising from the segregation of polar ionic headgroups and nonpolar alkyl domains. While scattering techniques such as SWAXS and neutron scattering have provided valuable structural insights, fluorescence-based molecular probes offer a powerful complementary approach for characterizing local microenvironments in ionic systems. In this study, we designed and synthesized a protic ionic liquid (PIL) that forms ionogels and exhibits liquid-crystalline ordering. To unravel the microstructural organization of the neat PIL, we used environment-sensitive dyes, Nile Red (NR) and Nile Blue Sulphate (NBS), and systematically investigated fluorescence intensity, anisotropy, and lifetime behavior. Microviscosity determined by fluorescence, in comparison with bulk viscosity, clearly confirms pronounced microheterogeneity and the presence of distinct microdomains within the PIL. These insights not only deepen our fundamental understanding of its molecular environment of PIL but also provide a foundation for the rational design of tailored PIL-based materials for diverse energy and optoelectronic applications.

## **PO-CYSA-02: Solvent-free Synthesis and Electrochemical Evaluation of MnNi-Layered Double Hydroxide as a Bifunctional Electrocatalyst for Alkaline Water Splitting**

**Ranjan S. Shetti and Nagaraj P. Shetti\***

*Center for Energy and Environment, School of Advanced Sciences, KLE Technological University, Hubballi-580031, Karnataka  
E-mail : npshetti@kletech.ac.in*

The quest for efficient and low-cost electrocatalysts for overall water splitting is critical for sustainable hydrogen production. Herein, a solvent-free and environmentally benign synthesis of manganese–nickel layered double hydroxide (MnNi-LDH) is presented and its bifunctional electrocatalytic performance toward the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in alkaline media is evaluated. Comprehensive structural characterisations confirmed a hydrotalcite-like layered framework with hydroxyl groups and interlayer carbonate species. BET analysis revealed a mesoporous texture facilitating the efficient electrolyte penetration and gas diffusion. Electrochemical evaluation demonstrated excellent OER activity, requiring only 187 mV overpotential at 10 mA cm<sup>-2</sup> with a low Tafel slope of 88 mV dec<sup>-1</sup>. For HER, MnNi-LDH delivered 225 mV overpotential at 10 mA cm<sup>-2</sup> with favourable kinetics. Notably, the catalyst exhibited long-term durability over 50 h under continuous operation, maintaining stable performance. A full water electrolyser using MnNi-LDH as both anode and cathode achieved 1.55 V at 10 mA cm<sup>-2</sup>, underscoring its practical feasibility. The Mn–Ni redox synergy promotes OH<sup>-</sup> adsorption and electron transfer, while the mesoporous nanosheets improve mass transport and gas release. Overall, this work integrates green synthesis with high electrocatalytic efficiency and durability, establishing MnNi-LDH as a promising bifunctional catalyst for sustainable hydrogen generation.

## **PO-CYSA-03: Tuning Supercapacitor Electrode Properties: Role of Hexagonal Boron Nitride in Graphene Amine Nanostructures**

**Bipin S. Chikkatti<sup>1</sup>, Ashok M. Sajjan<sup>1,2\*</sup> and Nagaraj R. Banapurmath<sup>2</sup>**

*<sup>1</sup>Department of Chemistry, KLE Technological University, Hubballi 580031*

*<sup>2</sup>Centre of Excellence in Material Science, School of Mechanical Engineering, KLE Technological University, Hubballi 580031*

This study presents the fabrication and electrochemical performance of a G-NH<sub>2</sub>/hBN nanocomposite as an advanced electrode material for supercapacitors. By integrating hexagonal boron nitride (hBN) into graphene amine (G-NH<sub>2</sub>), the nanocomposite demonstrates

enhanced capacitive behavior and stability. Structural and compositional analysis using Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Raman spectroscopy, Scanning Electron Microscopy (SEM) and Energy dispersive X-ray spectroscopy (EDS) confirmed the successful incorporation of hBN into the G-NH<sub>2</sub> matrix, promoting improved charge transport and surface interaction. Electrochemical characterization via Cyclic voltammetry (CV), Electrochemical impedance spectroscopy (EIS), Potentiodynamic polarization (PDP) and Galvanostatic charge-discharge (GCD) revealed that the G-NH<sub>2</sub>/hBN nanocomposite exhibited significantly enhanced capacitance and charge-transfer properties. GCD measurements reveal a specific capacitance of 203.68 F g<sup>-1</sup> at 0.75 A g<sup>-1</sup> which is considerably higher than values reported for graphene-related hBN composites. Long-term cycling demonstrates 86% capacitance retention over 10,000 cycles, showcasing excellent durability. The Ragone plot analysis shows that the G-NH<sub>2</sub>/hBN electrode delivers a high energy density of 102.12 Wh kg<sup>-1</sup> at a power density of 2850 W kg<sup>-1</sup>. These results suggest that the synergistic interaction between G-NH<sub>2</sub> and hBN significantly enhances electrochemical performance, making the nanocomposite a promising material for energy storage devices.

## **PO-CYSA-04: Carbon Alchemy: Lignite Transformed into High-Performance Graphite**

**Venkatesan Natesan<sup>1</sup>, Santhoshini Murugan<sup>1</sup>,  
Kothandaraman Ramanujam<sup>1,2,3\*</sup> and Mysore Sridhar Santosh<sup>4</sup>**

<sup>1</sup>*Clean Energy Laboratory, Department of Chemistry, Indian Institute of Technology Madras (IITM), Chennai 600036, Tamil Nadu*

<sup>2</sup>*The Energy Consortium, IIT Madras, Chennai 600036*

<sup>3</sup>*Centre for Future Materials, University of Southern Queensland, Australia*

<sup>4</sup>*CSIR-Central Institute of Mining and Fuel Research (CIMFR), Digwadih Campus, PO: FRI, Dhanbad, Jharkhand 828108*

*E-mail: gveen.sjc@gmail.com, rkraman@iitm.ac.in*

An earth-abundant and low-cost lignite coal was employed as a carbon precursor for the synthesis of highly pure synthetic graphite (SG) through carbonization, followed by high-temperature graphitization treatment at different temperatures (2800 and 3000 °C). The microstructural characteristics of the obtained SG material were systematically investigated using X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Raman spectroscopy, and nitrogen adsorption-desorption. The results reveal that the microstructures of SG-2800 and SG-3000 are strongly dependent on the graphitization temperature. The SG graphitized at 3000 °C has a perfectly ordered layered structure with a high degree of graphitization. The synthesized SG-3000 is used as an anode material

for a lithium-ion battery (LIB), giving a maximum reversible capacity of 305 mAh g<sup>-1</sup> at a current rate of 0.1C, along with superior rate capability and excellent cycling stability, retaining 94% of its initial capacity after 100 cycles. These findings highlight the potential of lignite coal as an inexpensive and scalable precursor for producing high-performance synthetic graphite suitable for advanced lithium-ion battery applications.

## **PO-CYSA-05: Concerted Deoligomerization and Inactive Reoligomerization of the Hexameric AAA+ Proteasomal ATPase Mpa upon Chemical and Thermal Perturbation**

**Pushpkant Sahu and Hema Chandra Kotamarthi\***

*Department of Chemistry, Indian Institute of Technology, Madras, 600036*

*E-mail: hchandra@smail.iitm.ac.in*

Protein oligomerization is essential for protein stability and function. The AAA+ ATPases are oligomeric enzymes that utilize ATP hydrolysis to drive various cellular processes, including protein degradation and DNA replication. In *Mycobacterium tuberculosis*, the proteasomal AAA+ ATPase, known as the Mycobacterial proteasomal activator (Mpa), forms a stable homohexamer even without nucleotides. Mpa comprises four domains: a Coiled-Coil (CC) domain, two oligonucleotide/oligosaccharide-binding domains (OB1 and OB2, collectively called the Inter-Domain or ID), and the AAA+ domain. The ID domain drives spontaneous oligomerization through strong non-covalent interactions. To investigate Mpa's oligomerization mechanism, we examined its response to chemical and thermal perturbation using spectroscopy, electrophoresis, calorimetry, and mass photometry methods. Chemical denaturation using urea, monitored using CD spectroscopy, tryptophan fluorescence, native PAGE, and single-particle mass photometry, revealed that Mpa directly converts from a hexameric state to an unfolded monomer without significantly populating other oligomeric states, indicating a concerted but non-cooperative pathway. Refolding of the unfolded Mpa led to a mixture of hexameric and monomeric species that are catalytically inactive. Thermal denaturation was investigated using CD, tryptophan fluorescence, differential scanning calorimetry (DSC), ATPase activity assays, and turbidity measurements. These analyses show that the Mpa hexamers unfold and spontaneously form amorphous aggregates at lower thermal stress, followed by dissociation to either partially folded or fully unfolded monomers, indicating a concerted and cooperative pathway. Collectively, these results indicate that Mpa is an obligate oligomer that follows distinct pathways during chemical

and thermal deoligomerization. The chemical perturbation transitions the Mpa hexamer to an unfolded monomer, and the thermal stress aggregates the protein, plausibly due to the exposure of hydrophobic residues.

### **PO-CYSA-06: Preparation and Characterization of PVA/CS Blend based Bioactive Films for the Application of Vegetable Packaging**

**Shiddalingesh G. Havanur and Ravindra B. Chougale**

*P. G. Department of Chemistry, Karnatak University, Dharwad-580 003, Karnataka*

*E-mail: chougaleravindra@yahoo.com*

This study aims to develop active agent-incorporated PVA and cationic starch active films through eco-friendly solution casting and solvent evaporation technique. FTIR and XRD studies reveals the intermolecular interactions between active agent, PVA and cationic starch, as well as the amorphous nature of the active biofilms. The active films show increased mechanical properties. The plasticizing effect of active agent caused decrease in hydration and barrier properties against water vapour and oxygen of the active films. However, the active films revealed enhanced antibacterial and antioxidant activity. Active films packed cherry tomatoes exhibits reduced weight loss. Furthermore, maintaining pH, total soluble solids and controls the total bacterial growth for up to 25 days of storage.

### **PO-CYSA-07: Electrochemical Sensing of the CNS Stimulant Drug using a Sulfur Doped g-C<sub>3</sub>N<sub>4</sub>/MWCNTs Hybrid Electrode: Insights into Analytical Applications**

**Harshitha A.<sup>1,2</sup> and Jyothi Abbar<sup>3</sup>**

<sup>1</sup>*Research Scholar, Visvesvaraya Technological University, Belagavi- 590014, Karnataka*

<sup>2</sup>*Department of Chemistry, Nitte Meenakshi Institute of Technology, Nitte (Deemed to be university), Bengaluru-560064, Karnataka*

<sup>3</sup>*BMS Institute of Technology and Management, Bengaluru 560064, Affiliated to Visvesvaraya Technological University, Karnataka*

Sulfur doped graphitic carbon nitride with multiwalled carbon nanotubes (S-doped gC<sub>3</sub>N<sub>4</sub>/MWCNTs) were used as a modified glassy carbon electrochemical sensor to detect psychostimulant drug, Mefexamide hydrochloride (MAH). The electrochemical activity was evaluated using surface characterization techniques along with electrochemical methods such as cyclic voltammetry (CV) and square wave voltammetry (SWV). The as modified sensor demonstrated a sensitive and selective response towards MAH, showed significantly

enhanced electrocatalytic activity in comparison to bare glassy carbon electrode (GCE) in phosphate supporting electrolyte of pH 7.0. The redox peaks seen in the cyclic voltammetry technique showed adsorption-controlled behavior. Under optimized SWV conditions for MAH detection, the limit of detection (LOD) and limit of quantification (LOQ) were found as 50.14 nM and 167.1 nM, respectively. The study systematically assessed the potential interference of various excipients in the analytical procedure for detecting MAH in complex matrices. The results demonstrated that the method was simple, reliable, and highly effective, enabling accurate detection of MAH in real samples such as water and biological fluids. These findings underscore the robustness and versatility of the approach, highlighting its potential for broad application in both environmental and clinical analysis.

### **PO-CYSA-08: Optical and Structural Properties of 4,4'-bis(9H-carbazol-9-yl) biphenyl (CRB)-Loaded $\alpha$ -Ray Irradiated Chitosan Films**

**Pushparekha<sup>1,2</sup>, Balladka Kunhanna Sarojini<sup>e\*</sup> and Bikrodi Sesappa Dayananda<sup>3</sup>**

<sup>1</sup>*Department of Chemistry, HKBK College of Engineering, Nagavara, Bangalore-560045*

<sup>2</sup>*Department of Chemistry, Mangalore University, Mangalagangothri-574199, Mangalore, Karnataka*

<sup>3</sup>*Department of Industrial Chemistry, Mangalore University, Mangalagangothri-574199, Mangalore, Karnataka*

<sup>e</sup>*E-mail: bksaroj35@gmail.com*

In present work, 4,4'-bis(9H-carbazol-9-yl) biphenyl (CRB) a hole transport material used in OLEDs was incorporated into chitosan films and were prepared by solvent casting technique. The dopant just intercalated physically in the matrix reflected by no notable changes in crystallinity. Even XPS also exhibited only a peak corresponding to -NH<sub>2</sub> group of chitosan at 400eV indicating that no chemical changes occurred during intercalation. The absorption behaviour complemented the similar trend with a red shift in  $\lambda_{\text{max}}$  changing from 301nm to 325nm with hyperchromism due to twisted nature of CRB dopant. The optical band gap of the films was in a range of 2.03-2.57eV. The photoluminescence property of these films showed interesting phenomenon of quenching in emission intensity upon irradiation at  $\lambda_{\text{max}}$  392nm (UVA region). The quenching of fluorescence could be attributed to the photo induced electron transfer from polaron of the matrix to the acceptor CRB and also affecting the microenvironment of matrix. The photoluminescence turnoff behaviour of chitosan/CRB (Guest-Host) composite films upon irradiation could be applied to fabricate a sensor device to detect ionizing radiations.



## **PO-CYSA-09: Development of ZnO/MWCNT@GCE for Electrochemical Investigation of Tartrazine – An Analytical Approach.**

**Suma J. G<sup>1,2</sup>, Rajappa S.K<sup>1\*</sup> and Sharanappa T. Nandibewoor<sup>3\*</sup>**

<sup>1</sup>Department of Chemistry, Karnatak Science College, Dharwad 580001

<sup>2</sup>Department of Chemistry, KLE Society's P C Jabin Science College, Hubballi-580031, Karnataka

<sup>3</sup>Department of Chemistry, School of Advanced Sciences, KLE Technological University, Hubballi-580031, Karnataka

E-mail: drrajappask@gmail.com; st.nandibewoor@kletech.ac.in

The Tartrazine (TTZ) also called as Acid Yellow 23, is a widely used synthetic dye in the food and cosmetic industry. Due to its potential health risk, its determination in a trace level is very much necessary. A voltametric method was developed for trace-level determination of TTZ using a Zinc Oxide/ Multiwall carbon nanotube composite (ZnO/MWCNT). The synthesised ZnO Nps were characterised by XRD, SEM with EDX and FTIR. Electrochemical impedance spectroscopy (EIS) was performed to check its enhanced catalytic activity. Cyclic voltammetry (CV) and square wave voltammetry (SWV) were used to study TTZ's electrochemical behaviour. Optimal performance was achieved in phosphate buffer (pH 8.0). The limit of detection (LOD) and limit of quantification (LOQ) were 2.21 nM and 7.39 nM, respectively. The sensor was successfully applied for the determination of various food items, water & environmental samples.

## **PO-CYSA-10: Viologen-Based Zn-Electrochromic Energy Storage Device with Polymer Electrolyte for Smart and Scalable Applications**

**Vansh Bhutani and Kothandaraman R.\***

Department of Chemistry, IIT Madras, Chennai-600 036

E-mail: rkraman@iitm.ac.in

Electrochromic energy storage devices combine optical modulation with charge storage, enabling the development of smart, energy-efficient technologies such as self-powered windows and adaptive displays. In this work, we report on a large-area viologen-based zinc electrochromic energy storage device (Zn-EESD) that realises both high optical contrast and excellent energy performance. A custom synthesised dihydroxyhexyl viologen, [DHHV][Br], was incorporated into a flexible polymer electrolyte composed of polyvinyl butyral, lithium perchlorate, and propylene carbonate to achieve high ionic conductivity and reversible redox behavior. Devices featuring this material exhibit vivid and reversible color changes from colorless to



deep blue, with a large optical modulation ( $\Delta T = 82.84\%$  at 603 nm) and high coloration efficiency of  $402.5 \text{ cm}^2 \text{ C}^{-1}$ . Paired with a Zn anode, the Zn-EESD demonstrated a self-coloration contrast of 92%, delivered  $86.06 \text{ mAh g}^{-1}$  discharge capacity, and maintained 95.25% energy efficiency. A larger  $5 \text{ cm}^2$  device retained an efficiency of 89.07%, and three connected cells successfully powered a 3 V LED for 120 minutes. This work demonstrates how designing polymer electrolytes in conjunction with molecular engineering can facilitate the scale-up of multifunctional electrochromic energy storage systems.

## **PO-CYSA-11: Development of Electron Donor-Acceptor Fluorophores Incorporating 2-(2-(Tert-Butyl)-6-Methyl-4h-Pyran-4-Ylidene)Malononitrile Frameworks for Sensing and Biological Studies**

**Gummadi Leela Prabha Anisha and Ravi Kumar Kanaparthi\***

*Department of Chemistry, Central University of Kerala, Tejaswini Hills, Periyar, Kasaragod, Kerala, 671316*

*E-mail: anisha.pch072203@cukerala.ac.in; rkchem@cukerala.ac.in*

Organic molecules with delocalized  $\pi$ -electrons are desirable candidates for developing functional materials for various applications. Organic -conjugated molecules are inexpensive to synthesize, and their structure-property relationship can be customized to our particular interests, making them ideal candidates in material science. To develop two new fluorescent sensors namely, AP-1 & AP-2 based on 2-(2-methyl-4H-chromen-4-ylidene)malononitrile and 2-(2-(tert-butyl)-6-methyl-4H-pyran-4-ylidene)malononitrile acceptors and conjugated  $\delta$ -systems is 4-(bis(pyridin-2-ylmethyl)amino)benzaldehyde as electron donors shows a turn ON-OFF fluorescence sensor for Zn(II) based on an intramolecular charge-transfer (ICT) mechanism. AP-1 and AP-2 were synthesized by following well-known chemical reactions such as Vilsmeier-Haack formylation and Knoevenagel condensation. And also, AP-1 & AP-2 bind with zinc metal chelation. Since zinc has more biological importance. Furthermore, these molecules have been characterised using FT-IR, TGA, HRMS, and  $^1\text{H-NMR}$  spectroscopy. Photophysical properties were studied systematically using a UV-visible spectrophotometer and spectrofluorometer. Results show that the two molecules are thermally stable and exhibit strong absorption characteristics in the UV-visible region (250-650nm) and strong fluorescence characteristics in the 400-800nm region in various solvents. Further, upon screening for the detection of different metal ions, these molecules sense selectively for Zinc ions. The zinc ion detection is visible to the naked eye.

## **PO-01: Physical Chemistry Perspectives on Biocompatible Lipid Nanocarriers for Therapeutic Delivery**

**Paurnima Talele**

*Shri Guru Gobind Singhji Institute of Engineering and Technology,  
Nanded-431606 (M.S.)  
E-mail: talelepaurnima@gmail.com*

Lipid nanocarriers provide a biocompatible and tunable platform for therapeutic delivery, where performance depends on self-assembly, molecular packing, and drug-lipid interactions. From the standpoint of physical chemistry, characterization techniques are central to unraveling the relationship between nanoscale structure and function. Light scattering techniques along with microscopic techniques, offer assessment of particle size, polydispersity, and colloidal stability, parameters that critically determine biodistribution and drug release. Differential scanning calorimetry (DSC) probes lipid phase transitions, polymorphism, and crystallinity, revealing how enthalpic and entropic factors govern packing, drug incorporation, and release kinetics. Isothermal titration calorimetry (ITC) complements these insights by directly quantifying binding thermodynamics, providing enthalpy, entropy, and affinity constants that describe hydrophobic, electrostatic, and hydrogen-bonding contributions to drug partitioning in lipid domains. Structural resolution is achieved through X-ray diffraction (XRD), and fluorescence spectroscopy captures dynamic aspects of the lipid environment, including bilayer fluidity, polarity, and heterogeneity, offering real-time insight into drug localization and carrier microenvironments. My talk will show how physical chemistry approaches uncover the thermodynamic and structural principles that both govern lipid nanocarrier behavior and enable their rational design as stable, biocompatible systems for controlled drug release.

## **PO-02: Studies of Adiabatic compressibility and Acoustic impedance of Drug Phenobarbital Sodium in Aqueous Solution at Different Temperatures**

**Sachin B. Ingole**

*Department of Chemistry, S.B.E.S College of Science, Chh. Sambhajinagar,  
Maharashtra*

The Density ( $\rho$ ), ultrasonic velocity (U), and viscosity ( $\eta$ ) measurements have been carried out for Phenobarbital sodium in aqueous solution having different concentrations at temperatures of 298.15K, 303.15K, 308.15K and 300.15K. Experimental data have been used to estimate the adiabatic compressibility ( $\beta$ ) and acoustic

impedance (Z). The results are discussed in terms of structure-making (or) structure-breaking effects of drug molecules in the mixtures.

### **PO-03: Thermodynamic Profiling of Peptide Backbone Units and Protein Model Compounds in Ammonium based Ionic Liquids**

**T. Vasantha**

*Department of Chemistry, Sri Venkateswara College, University of Delhi,  
Dhaura Kuan, New Delhi-110021  
E-mail: vasanthathoti@gmail.com, tvasantha@svc.ac.in*

This research investigates the thermodynamic and structural effects of ammonium-based ionic liquids (ILs) on protein model compounds, focusing on their role as co-solvents in protein folding and stability. Protein folding/unfolding is highly sensitive to the surrounding environment, and co-solvents can either stabilize or destabilize the native structure. ILs have emerged as promising co-solvents due to their tuneable properties and growing applications in biochemical processes.

To understand how ILs influence biomolecular interactions, solubility measurements were conducted at 25/ °C across varying IL concentrations. These measurements involved glycine-based peptides (Gly, Gly, , Glyf , Gly,, , cyclic glycylglycine) and a range of amino acids (Ala, Val, Leu, Trp, Tyr, Phe, His, Thr, Gln, Ser) in aqueous solutions containing six different ILs: DEAA, DEAS, TEAA, TEAS, TEAP, and TMAA.

The transfer free energy ( $\Delta G_{tr}$ ) values from water to ILs were predominantly positive for glycine peptides, indicating unfavourable interactions between ILs and peptide surfaces. This exclusion effect suggests that ILs do not penetrate the peptide structure, thereby promoting its stability. Similarly, amino acids such as Ala, Val, Leu, Trp, and Tyr showed decreased solubility with increasing IL concentration, consistent with a salting-out effect and unfavourable IL-AA interactions.

Interestingly, amino acids like His and Ser also exhibited positive  $\Delta G'_{tr}$  values, while Phe, Thr, and Glu displayed both positive and negative values depending on the IL type, highlighting the nuanced nature of these interactions. These findings collectively demonstrate that alkyl ammonium ILs act as stabilizing agents for protein model compounds, primarily through exclusion mechanisms. Moreover, the alkyl chain structure of the ILs plays a significant role in modulating these interactions and the overall stability of the biomolecules.

## **PO-04: Multi-Target Drug Design is More Beneficial than Single Target**

**Abhay Krishna<sup>1</sup> and Ajay Kumar Yadav<sup>2</sup>**

<sup>1</sup>*Department of Applied Sciences & Humanities, K. M. C. Language University Lucknow (U.P)*

<sup>2</sup>*Department of Chemistry, K. M. C. Language University Lucknow (U.P)*  
*E-mail: abhaykrishna@knclu.ac.in*

Multi-target drug design (MTDD) represents a paradigm shift from the traditional single-target approach in pharmaceutical research. Unlike conventional drugs that act on one specific molecular target, MTDD aims to modulate multiple biological pathways or receptors simultaneously. This strategy is particularly advantageous in the treatment of complex, multifactorial diseases such as cancer, neurodegenerative disorders, cardiovascular diseases, and metabolic syndromes, where pathological processes involve interconnected networks rather than isolated mechanisms. By addressing multiple targets, MTDD can enhance therapeutic efficacy, reduce the likelihood of drug resistance, and achieve synergistic effects, ultimately improving patient outcomes. Advances in computational biology, systems pharmacology, and high-throughput screening have accelerated the rational design of multitarget agents, allowing for the optimization of pharmacodynamic and pharmacokinetic profiles. Overall, MTDD offers a promising and holistic approach to modern drug discovery, aligning with the growing understanding of disease complexity and personalized medicine.

## **PO-05: Anti-Gravity Drop Motion and Co-Solute Transport on Special Wetting Surfaces**

**Vickramjeet Singh**

*Department of Chemistry, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar 144008, Punjab*  
*E-mail: singhvj@nitj.ac.in*

Modulation of surface wettability plays a vital role in controlling droplet dynamics for applications in microfluidics, self-cleaning surfaces, and biomedical devices. A particularly intriguing phenomenon is droplet motion against gravity, driven by interfacial tension gradients. In this study, we demonstrate a simple strategy to induce spontaneous horizontal and uphill motion of tetrahydrofuran (THF) droplets without external stimuli. A binary non-aqueous mixture of volatile THF and hexamethyldisilane (HMDS) exhibited self-propelled movement on fully wetting glass surfaces, successfully climbing a tilt of  $\sim 10^\circ$ . The observed motion arises from Marangoni stresses generated by solute concentration gradients within the evaporating binary droplet.

Additionally, this system enabled transport of dissolved solutes along the direction of motion. The results highlight a minimalistic and efficient approach to achieving gravity-defying droplet motion, offering promising potential for microfluidic manipulation, passive liquid transport, and surface engineering applications.

### **PO-07: Solid-State Kinetic And Thermal Studies of an Iron(III) Complex with Schiff Base Derived From 5-Anilino-1,2,3,4-Thiatriazole**

**Sarita Prasad**

*Department of Chemistry, R.N. College, Pandaul, Madhubani, Bihar-847234  
E-mail: sarita13478@gmail.com*

The synthesis and thermal behavior of an iron (III) complex with the Schiff base derived from 5-anilino-1,2,3,4-thiatriazole (ATT) were investigated. The formula  $[\text{FeL}_2\text{Cl}] \text{Cl}$  with a molecular weight of 520.25 mg was validated by elemental analysis. Three stages of decomposition were identified by thermogravimetric analysis: the ligand broke down between 200 and 250 °C, moisture and chloride ions were removed between 100 and 200 °C, and  $\text{Fe}_2\text{O}_3$  was formed at about 260 °C.

Freeman-Carroll and Zsako's modified Doyle methods were used to perform a kinetic analysis of the second stage. With an activation energy of roughly 12–13 kcal mol<sup>-1</sup> and a reaction order near zero ( $n \approx 0.1$ ), both demonstrated good agreement. At 523 K, the entropy of activation was  $\Delta S^\ddagger = -210.65$  e.u., and the frequency factor was determined to be  $1.02630 \times 10^2 \text{ s}^{-1}$ , indicating a highly ordered transition state. The study highlights the predictable decomposition pathway and provides useful insight into the solid-state kinetic parameters and stability of the  $[\text{FeL}_2\text{Cl}_2]\text{Cl}$  complex.

### **PO-06: Highly Sensitive and Colorimetric Detection of Mercury Ions in Water**

**R. Surya Sekhar Babu and Ravi Kumar Kanaparthi\***

*Department of Chemistry, Central University of Kerala, Tejaswini hills, Periyar, Kasaragod, Kerala, 671316  
E-mail: rayudu.2301107009@cukerala.ac.in; rkchem@cukerala.ac.in*

Mercury is one of the highly toxic, bio-accumulating, and hazardous heavy metals that have adverse effects on various life forms. These adverse effects include enhanced risk for severe brain damage, kidney problems, immune dysfunction and motion disorders in humans. Considering the significance of mercury detection, a new molecular system B-1 has been designed and synthesized from carbamodithioate-based conjugated 1,3 Indanedione molecule-based sensor (B-1) for

selective and rapid detection of mercury ( $\text{Hg}^{2+}$ ) in drinking water has been proposed. The B-1 molecule was synthesized by chemical reactions such as Vilsmeier-Haack and Knoevenagel condensation—further characterized by FT-IR, Mass spectrometry, NMR spectroscopy and Single crystal XRD. In addition, photophysical properties were studied systematically using a UV-visible spectrometer and spectrofluorometer and TGA analysis was performed. Results showed that the sensor was thermally stable and exhibited strong absorption characteristics in the UV-visible region (200-550nm) and strong fluorescence in the range of (400-650nm). The sensor responds with a  $\text{Hg}^{2+}$  coordination interaction between (B-1) and  $\text{Hg}^{2+}$ . The thiol- $\text{Hg}^{2+}$  interaction was studied by fluorescence spectroscopy (bulk solutions) of (B-1) with increased concentrations of  $\text{Hg}^{2+}$  (10 nM to 30  $\mu\text{M}$ ). The sensor's specificity in the presence of other interfering metals like  $\text{Pb}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Na}^{2+}$ ,  $\text{Ag}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Pd}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Sn}^{2+}$  and  $\text{Cd}^{2+}$  has been determined. The sensor can be used as a highly sensitive, selective, portable, real-time, on-site  $\text{Hg}^{2+}$  optical probe for drinking water. We shall present photophysical studies as well as sensing applications of the new molecule, B-1.

## **PO-08: Voltammetric Determination of Thymol By A Modified Carbon Paste Electrode**

**H.R. Sahana and Y. Arthoba Nayaka\***

*Department of Chemistry, School of Chemical Sciences, Kuvempu University, Shankaraghatta-577451, Karnataka*

*E-mail: drarthoba@gmail.com, sahanahr0101@gmail.com*

The synthesised cerium-doped  $\text{Fe}_2\text{O}_3$  nanoparticles were used to develop a modified electrochemical sensor based on a carbon paste electrode (CPE) for the voltammetric determination of thymol(TML). The synthesised  $\text{Fe}_2\text{O}_3$  and Ce-doped  $\text{Fe}_2\text{O}_3$  NPs were characterized using XRD, FESEM with EDX, and TEM techniques. The average crystalline size of the synthesized nanoparticles has been found to be 19 to 30 nm. The Ce- $\text{Fe}_2\text{O}_3$  modified carbon paste electrode (Ce- $\text{Fe}_2\text{O}_3$ /CPE) exhibits superior electrochemical performance towards the oxidation of TML as compared to the  $\text{Fe}_2\text{O}_3$ /CPE. The Ce- $\text{Fe}_2\text{O}_3$ /CPE exhibited a linear response towards the detection of TML under investigational conditions, with a detection limit of  $1.4052 \times 10^{-8} \text{M L}^{-1}$ . The various parameters such as heterogeneous rate constant ( $k^\circ$ ), number of electrons transferred ( $n$ ), electroactive surface area of the electrode ( $A$ ), and charge transfer resistance ( $R_{ct}$ ), have been calculated. The sensitivity, long-term stability, and reproducibility of the developed sensor were estimated. The analytical validity of the developed electrode has been examined through the real sample analysis using a soil sample.

## **PO-09: Structure–Efficiency Relationship in DSSCs: A Study of Auxiliary Donors, Acceptors, and $\pi$ -Spacers in D-A- $\pi$ -A Sensitizers**

**Prabhakar Chetti**

*Department of Chemistry, National Institute of Technology (NIT),  
Kurukshetra-136119  
E-mail: chetti@nitkkr.ac.in*

One of the main constituents of a dye sensitized solar cell (DSSC) that influences its efficiency to transform solar energy into electrical energy is the photosensitizer or the dye. Thus, the choice of donor,  $\pi$ -bridge and the acceptor is very crucial while designing the dye's architecture. In the present work, the influence of donor, acceptor and  $\delta$ -spacer in the basic D-A- $\pi$ -A structure of organic dye has been investigated. Geometry, charge transfer, photovoltaic and optoelectronic properties of the proposed molecules have been studied. Further, the dyes were adsorbed on the nanocrystalline surface of the semiconductor ( $\text{TiO}_2$ ). Theoretical evaluation of various parameters such as energy gap between frontier molecular orbitals (FMOs), electron affinity, ionization potential, reorganization energy has been executed using density functional theory (DFT) and time dependent density functional theory (TD-DFT). Overall power conversion efficiency (PCE) of the designed molecules has been simulated by using all the photovoltaic parameters. Thus, this study shows that variation in the basic structure of dye can be helpful in fine-tuning the overall performance of a DSSC.

## **PO-10: Efficient Recovery of Rare Earth Metal Ions Using Lidocaine-Based Solvent Mixtures**

**M. Shaibuna and Ramesh L. Gardas\***

*Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036  
E-mail: gardas@iitm.ac.in*

Rare earth elements (REEs), particularly lanthanides, are critical to advanced technologies due to their unique magnetic, luminescent, and electrochemical properties. They play indispensable roles in electronics, LEDs, and other high-performance devices, as well as in strategic sectors such as national defence, energy, metallurgy, and petrochemicals. However, limited natural reserves and increasing demand have intensified the need for sustainable recovery and recycling methods. This study investigates the extraction of REEs using lidocaine–nonanoic acid mixtures at various molar ratios. The mixtures were characterised using spectroscopic and thermal analyses, and their physicochemical properties, including density and viscosity, were evaluated over a range of temperatures. Liquid–liquid extraction



experiments were conducted to optimise parameters such as metal ion concentration, volume ratio, and pH. The optimised system exhibited high extraction efficiency, while stripping and reusability tests confirmed the potential of these mixtures for sustainable REE recovery. Overall, the findings demonstrate an environmentally friendly and efficient approach for recycling rare earth metals from secondary sources, supporting circular economy initiatives.

### **PO-11: Hydrophobic Deep Eutectic Solvents for Sustainable and Efficient Removal of Anionic Dyes**

**Devika S. R. and Ramesh L. Gardas\***

*Department of Chemistry, Indian Institute of Technology Madras, Chennai- 600036  
E-mail: gardas@iitm.ac.in*

The textile industry faces a critical environmental challenge arising from the discharge of dyeing effluents enriched with hazardous dyes and auxiliary chemicals into aquatic ecosystems. The persistence of these contaminants poses severe ecological and sustainability concerns, underscoring the necessity for efficient and sustainable removal strategies. Conventional treatment methods, however, are often inadequate for the complete elimination of such stable and complex pollutants. In the present study, the effective removal of two anionic dyes, cresol red (CR) and methyl orange (MO), was explored using a hydrophobic deep eutectic solvent (DES) via liquid-liquid extraction (LLE). The extraction parameters were systematically optimized by evaluating the influence of diluent type, extractant concentration, and equilibration time. Furthermore, the efficiency of various stripping agents and stripping phase ratios was critically assessed to establish the optimal extraction conditions. The regenerated solvent was subsequently employed in successive extraction cycles to evaluate its reusability and stability.

### **PO-12: Host-guest Complexes of $\alpha$ -cyclodextrin and Novel Triazole Based Ionic Liquid as Nitrogen-Doped Carbon Precursor for High Performance Supercapacitors**

**Sumana Brahma, Ramesh L. Gardas\* and Kothandaraman Ramanujam\***

*Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036  
E-mail: gardas@iitm.ac.in, rkraman@iitm.ac.in*

Developing high-performance supercapacitors (SCs) with long cycle life using sustainable materials is paramount for next-generation energy storage technologies. Nevertheless, achieving a high specific capacitance while preserving superior energy density and excellent cycling stability remains a significant challenge. To enhance the

performance of electrode material, the extensively used schemes are increasing the surface area by chemical activation. Here, we proposed a simplistic and effective approach to develop nitrogen-doped activated carbon (AC) materials by introducing environmentally benign host-guest inclusion complexes (ICs) precursors, with cyclodextrin (CD) and Ionic liquids (ILs). The Insertion of heteroatom- comprising guest molecules, such as nitrogen-enriched ILs, in the cavity of host molecules  $\beta$ -CD not only doped the carbon skeleton with nitrogen but also upgraded the carbonization yield. The excellent performance of ICs derived ACs is attributed to the faradaic charge contribution as the surface of the carbons are influenced by the nitrogen source and the type of oxygen functional groups present on the surface. Further, the nitrogen-doped ACs demonstrated excellent performance as SCs electrode material with maximum specific capacitance ( $258\text{ F g}^{-1}$ ) at  $0.5\text{ A g}^{-1}$  in aqueous electrolyte. These findings inspire further efforts to optimize the system toward the development of high-performance and environmentally friendly energy storage devices.

### **PO-13: Evaluation of Conductive, Thermo-pH Responsive Smart Polymer-Based Films**

**Radha Doddamani**

*Department of Chemistry, Karnatak University Dharwad*  
*E-mail: radhadoddamani@gmail.com*

Although Mother Nature provides many inspirations for designing and developing new materials, creating synthetic systems capable of responding to stimuli in a controllable and predictable fashion represents significant challenges. In this context, the smart polymers known as stimuli-responsive polymers which change their properties such as shape, surface, permeability, optical properties and electrical properties upon external stimuli such as temperature, electric field,  $p^H$ , light, magnetic field, electrical field, glucose etc. This study aims to develop conductive yet stimuli responsive flexible polymeric films. Interpenetrating network (IPN) of polyaniline (conductive polymer) in polyvinyl alcohol network and chitosan ( $p^H$  responsive), poly-iso-N-acrylamide IPN (thermoreponsive) network into polyvinyl alcohol further these were blended and crosslinked with glutaraldehyde. The physicochemical properties of the resulting blend films were investigated. Films have shown excellent shape memory performance towards change in  $p^H$  and temperature. The electrochemical performance of all the films was evaluated by cyclic voltammetry for instance at  $50\text{ mVs}^{-1}$  scan rate films have shown specific capacitance nearly about  $319\text{ Fg}^{-1}$ . Furthermore, these films can have applications as electrode materials for flexible light-weight smart micro-

supercapacitor devices, as smart wearables as patches and as smart indicators in food packaging applications.

#### **PO-14: Spectrophotometric Kinetics and Mechanistic Insights into Osmium (VIII) Catalyzed Oxidation of Aspirin by Hexacyanoferrate (III) in Alkaline Medium - A Mechanistic Pathway**

**Beena Gupta and Riya Sailani\***

*Department of Chemistry, Centre of Advanced Studies, University of Rajasthan, Jaipur, Rajasthan-302004*  
*E-mail: l.p.\_riya@yahoo.co.in*

The kinetics of aspirin oxidation by hexacyanoferrate (III) in alkaline medium, catalyzed by osmium (VIII), were systematically investigated. The reaction exhibits first-order dependence on both the oxidant and catalyst, with hydroxide ion and aspirin exerting complex effects on the rate. A suitable rate law was derived, and kinetic parameters were evaluated under various conditions. Activation and thermodynamic parameters were obtained using Arrhenius and Eyring equations. Solvent effects were extensively studied, revealing significant influence on reactivity. A plausible mechanistic pathway was proposed, further substantiated by Density Functional Theory (DFT) calculations at the B3LYP/6-311G(d,p) level, which showed strong agreement between experimental kinetics and computed energy barriers. These results provide compelling support for the proposed mechanism.

#### **PO-15: Development of Fe<sub>2</sub>O<sub>3</sub>/RGO Nanocomposite Infused with CTAB Surfactant Modified Glassy Carbon Electrode for Electrochemical Detection of Promethazine Hydrochloride in Real Samples**

**Amruta Patri<sup>1</sup>, Sharanappa T. Nandibewoor<sup>2</sup> and Ravindra R. Kamble<sup>1\*</sup>**

*<sup>1</sup>Department of Studies in Chemistry, Karnatak University Dharwad-580003*  
*<sup>2</sup>Department of Chemistry, School of Advanced Sciences, KLE Technological University, Hubballi, 580031, Karnataka*  
*E-mail: amrutapatri123@gmail.com*

In this study, we developed a metal oxide-reduced graphene oxide (RGO) nanoparticles-modified glassy carbon electrode (Fe<sub>2</sub>O<sub>3</sub>/RGO/CTAB@GCE) to facilitate a simple, sensitive, and efficient carbon-based sensor for the trace-level detection of an antihistamine drug promethazine hydrochloride (PMH). Fe<sub>2</sub>O<sub>3</sub> and RGO nanocomposites were created by hydrothermal and chemical processes respectively, the synthesised samples were characterised using Fourier-transform infrared spectroscopy, X-ray diffraction, scanning electron microscopy

and atomic force microscopy. Electrochemical impedance spectroscopy (EIS) assessed material performance. We used cyclic voltammetry (CV) and square wave voltammetry (SWV) to study the electrochemical behaviour and detection of PMH at the  $\text{Fe}_2\text{O}_3/\text{RGO}/\text{CTAB}/\text{GCE}$ . Outstanding catalytic characteristics, a large electroactive surface area, excellent absorptivity, and synergistic electrochemical activity for promethazine oxidation were demonstrated by the  $\text{Fe}_2\text{O}_3/\text{RGO}/\text{CTAB}/\text{GCE}$ . To create an electrochemical sensor with excellent performance, the electrolyte pH,  $\text{Fe}_2\text{O}_3/\text{RGO}/\text{CTAB}$  nanocomposite quantity, preconcentration potential (vs.  $\text{Ag}/\text{AgCl}$ ), and duration were all tuned. Under ideal circumstances, the suggested sensor showed linear concentration variations between  $0.6 \text{ nmol L}^{-1}$  and  $0.01 \text{ }\mu\text{mol L}^{-1}$ . The limits of detection and quantitation were  $0.36$  and  $1.21 \text{ nmol L}^{-1}$  respectively. The proposed sensor demonstrated high sensitivity, quick evaluation, outstanding repeatability and reproducibility. This innovative technique was successfully applied to measure PMH in urine and water samples.

## **PO-16: Drug-Deep Eutectic Solvent Interactions in Aqueous Solution: Volumetric Studies**

**Shikha Indoria<sup>1</sup>, Vickramjeet Singh<sup>2\*</sup>, Arpita Padhan<sup>2</sup> and Anshuman Pattanvall<sup>2</sup>**

<sup>1</sup>*Department of Chemistry, Government College Ropar, 140001*

<sup>2</sup>*Department of Chemistry, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar 144027, Punjab*

<sup>\*</sup>*E-mail: shivanya1316@gmail.com; shikha087@yahoo.com*

Deep eutectic solvents (DESs) have emerged as promising eco-friendly alternatives to traditional solvents. Gaining insight into their solution chemistry is essential for advancing green chemistry applications and pharmaceutical formulations. This study presents a detailed volumetric analysis aimed at elucidating the molecular interactions and thermodynamic behavior of theophylline in aqueous DES systems. A DES composed of PEG-400 and citric acid or ascorbic acid was designed to explore theophylline–DES interactions. Density and speed of sound measurements were carried out over the temperature range of  $293.15\text{--}318.15 \text{ K}$  at  $0.1 \text{ MPa}$ . The evaluation of apparent molar volumes, infinite dilution partial molar volumes, and volumetric transfer parameters revealed meaningful insights into theophylline–DES–water interactions. The results highlight a complex network of interactions between the DES components and theophylline, with dimerization of theophylline contributing to a decrease in transfer volume. Overall, this study enhances the understanding of DES-mediated drug–solvent interactions and provides valuable implications for pharmaceutical and green chemistry applications.

## PO-17: Enhancing the Properties of High Entropy Oxide (HEO) by Varying the Concentration of Constituent Metal Oxides: First Principles Studies

Mansingh Yadav and Yamini Sudha Sistla\*

*Department of Chemical Engineering, Shiv Nadar Institution of Eminence,  
Delhi NCR*

*\*E-mail: yamini.sistla@snu.edu.in*

High entropy oxides (HEO), the complex oxides consisting of five or more metal cations, have received substantial attention since a decade due to their exceptional properties such as high strength, thermal stability, wear, oxidation and corrosion resistance with advanced and tunable properties. During the design stage of new HEOs, the traditional trial and error experiments are resource, economic and energy intensive. The first principles methods are cognitive approaches which accelerate the material research from fundamentals. The structural, electronic, mechanical, and thermal properties of a novel and new  $\text{MO}_2$  (M= Ti, Zr, Ce, Mo, Mn) type HEO were evaluated for seven different atomic fractions of metal cations. Present study establishes the effect of concentration of constituent metal oxides of Ti, Zr, Ce, Mo, Mn on the overall properties of HEOs through first principles calculations. The elastic constants calculated using strain-stress method were used to compute the mechanical properties such as bulk modulus, shear modulus, Young's modulus, hardness, sound velocity, and thermal properties such as Debye temperature, thermal capacity and minimum thermal conductivity. The results of the current study conclude that, having unequal mole fractions of M in  $\text{MO}_2$ , would significantly enhance the density (5.431 to 5.839  $\text{g/cm}^3$ ) and hardness (6.48 to 9.50 GPa) of the HEOs as compared to equal metal cation concentrations. This strongly signifies the enhancement in mechanical stability of the non-equiatomic  $\text{MO}_2$  HEOs. The bulk modulus of the seven  $\text{MO}_2$  HEOs studied was in the range of 146.2 – 204.5 GPa suggesting improved deformation resistance to volume changes under stress by varying the metal concentrations. The HEOs exhibited low shear modulus (62.10 GPa - 91.2 GPa) indicating that these oxides are flexible and easily deformable. Furthermore, the  $\text{MO}_2$  HEOs showed Young's modulus values of 163.40 – 238.2 GPa and fracture toughness in the range of 1.38 - 1.90  $\text{MPa}\cdot\text{m}^{1/2}$ . The HEOs exhibited minimum thermal conductivity of 1.38 -1.69  $\text{W/m}\cdot\text{K}$  as obtained from Cahill's model (Fig. 1 (b)) indicating their potential application in thermal barrier coating. Among the seven  $\text{MO}_2$  HEOs studied, HEO-2 ( $\text{Ti}_2\text{Ce}_2\text{Zr}_6\text{Mo}_5\text{Mn}_5\text{O}_{40}$ ) displayed high hardness and fracture toughness and low minimum thermal

conductivity which has potential to attract extensive attention in thermal insulation and high temperature applications. The Ti, Ce, Zr, Mo and Mn based HEOs studied in the present work displayed better elastic moduli, sound velocity, Debye temperature, thermal capacity and minimum thermal conductivity as compared to the HEOs reported in literature. The anisotropy of ( $AX_2$ ) was also evaluated based on the 3-dimensional directional variation of elastic moduli.

## **PO-18: Fabrication of Ni-Fe-sulphides/Ni Foam Supercapacitor Electrodes for Enhanced Charge Storage and Energy Density.**

**Vaishnavee Kasar<sup>1,2,4</sup>, Suresh Shendage<sup>1</sup> and Ashis Kumar Satpati<sup>2,3\*</sup>**

<sup>1</sup>*Department of Chemistry, KET's V. G. Vaze Kelkar College, Mulund (E), Mumbai-400081*

<sup>2</sup>*Analytical Chemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085*

<sup>3</sup>*Homi Bhabha National Institute, Anushaktinagar, Mumbai-400094*

<sup>4</sup>*Vaishnavee Kasar worked as project trainee in Analytical Chemistry Division, Bhabha Atomic Research Centre during the course of the work*  
E-mail: [asatpati@barc.gov.in](mailto:asatpati@barc.gov.in); [vaishnaveekasar@gmail.com](mailto:vaishnaveekasar@gmail.com)

Transition metal sulfides are emerging as promising materials for supercapacitor electrodes due to their rich redox activity and favorable electronic conductivity. In this study,  $NiFe_2S_4$  was electrodeposited onto nickel foam via cyclic voltammetry (CV), exploiting the synergistic redox behavior of Ni and Fe ions to enhance charge storage. Initial electrochemical evaluation using CV, galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS) revealed a significant decline in specific capacitance over successive cycles, attributed to poor interfacial adhesion and surface contamination of the nickel foam. To overcome this, the substrate was pre-treated with concentrated  $H_2SO_4$  to remove native oxides and impurities, restoring surface reactivity and porosity. Post-treatment electrodeposition yielded a homogeneously coated, structurally stable  $NiFe_2S_4$  layer. Electrochemical analysis showed a marked improvement in specific capacitance ( $>700\text{ F/g}$ ), enhanced cycling stability, and reduced charge-transfer resistance. CV plots at varying scan rates demonstrated proportional current enhancement, indicating reversible ion diffusion during charge–discharge. Sustained discharge times at higher current densities further confirmed improved active site accessibility. These results highlight the importance of substrate conditioning in achieving reproducible, high-performance electrodes. The optimized  $NiFe_2S_4$ /Ni foam composite offers a cost-effective and electrochemically robust solution for next-generation supercapacitor applications.



## **PO-19: Wetting Modulation of Acrylamide–Acrylic Acid Membranes Embedded with PIL for Efficient Under-Oil Water Recovery**

**Arpita Padhan and Vickramjeet Singh\***

*Department of chemistry, Dr. B. R. Ambedkar National Institute of Technology,  
Jalandhar 144008, Punjab  
E-mail: singhvj@nitj.ac.in*

The release of oily wastewater from industrial activities and household sources poses serious environmental challenges, endangering valuable natural resources and threatening the survival of aquatic life. As a result, the separation of oil/water mixtures and stable emulsions has become a significant global concern. Acrylamide/acrylic acid-based gels were prepared by incorporating EAAC protic ionic liquid. Using APS as the initiator and NMBA as the crosslinker. The gels were optimised on the basis of swelling. The gels were characterised by FT-IR and PXRD analysis. FE-SEM analysis was conducted for morphological observation of the prepared membranes. By simply incorporating a protic ionic liquid, the synthesised gel demonstrated a very high swelling ratio in the case of acrylic acid gel. Considering their high swelling ability, the gels were employed for the absorption of water in the surrounding oil, as well as the absorption of dye from water. The gels were further subjected to wetting characterisation, depicting distinct behaviour in water and air surroundings.

## **PO-20: Protease-Dependent Selectivity in the Knotted Protein Degradation**

**Soham Mukherjee and Hema Chandra Kotamarthi\***

*Department of Chemistry, Indian Institute of Technology, Madras, 600036.  
E-mail: hchandra@smail.iitm.ac.in*

Knotted protein is a special class of protein where self-entanglement of the polypeptide chain results in a folded protein with a knot. Depending upon the knot topology, knotted proteins are classified as trefoil knotted ( $3_1$ ), figure of eight knotted ( $4_1$ ), gordian knotted ( $5_2$ ), and stevedore knotted ( $6_1$ ) proteins.

These proteins currently populate almost 1% of known protein structures in the PDB. However, the mechanism by which a protein folds with a knot and the functional significance of a knot in a protein remain elusive. Following initial reports of knots providing proteins with mechanical stability against cellular degradation by ATP-dependent proteases and proteasomes, we have tried to understand the degradation mechanism of model knotted protein substrates (CA



IX, miRFP709 and UCHL1) by proteases ClpXP and ClpAP and proteasomal system Mpa-20S CP, using steady-state fluorescence loss assay and SDS-PAGE densitometry assays.

ClpAP and ClpXP are known to be comparable in terms of their protein degradation activity. However, to our surprise, when degraded from the C to N terminus, ClpAP fails to degrade knotted proteins, whereas ClpXP degrades them very easily. To reconcile such unanticipated behaviour, we hypothesised that the flexibility of the protease's inner chamber plays a crucial role in the differential behaviour of these proteases and tested their flexibility by using covalently linked Arc-ssrA dimers. Proteasome Mpa-20S CP quite easily degrades knotted proteins from N to C terminal.

Thus, our study suggests that knots may contribute to protein stability against certain degradation systems, such as ClpAP. However, knotted proteins are still susceptible to degradation by other systems, including ClpXP and Mpa-20S CP. This duality could reflect evolutionary selection, where knots provide protection from some quality control mechanisms while retaining alternative pathways for maintaining protein homeostasis within the cell.

## **PO-21: Optimizing the Composition of (TiNbHfTaW) $C_2$ High Entropy Carbide Ceramic for Superior Mechanical Stability: Density Functional Theory**

**Nabila Tabassum and Yamini Sudha Sistla\***

*Department of Chemical Engineering, Shiv Nadar Institution of Eminence, Greater Noida, U.P.*

*E-mail: yamini.sistla@snu.edu.in*

High Entropy Ceramics (HEC) are a novel class of ceramic materials, known for their excellent thermo-mechanical stability, super hardness (> 40GPa) & corrosion resistance making them promising materials for industrial applications. Present study provides comprehensive evaluation of the effect of atomic concentrations of constituent metals on the structural, electronic, magnetic, mechanical and thermal properties of carbide-based HEC ((TiNbHfTaW) $C_2$ ) using density functional theory (DFT). Around 18 compositional variations such as (Ti<sub>0.2-x</sub>)(Nb<sub>0.2+x</sub>)HfTaWC, (Ti<sub>0.2-x</sub>)Nb(Hf<sub>0.2+x</sub>)TaWC, and (Ti<sub>0.2-x</sub>)NbHf(Ta<sub>0.2+x</sub>)WC, and (Ti<sub>0.2-x</sub>)NbHfTa(W<sub>0.2+x</sub>)C where x = 0.05, 0.1 and 0.15 were investigated. Among the compositions studied, Ti<sub>0.05</sub>Ta<sub>0.35</sub>Nb<sub>0.2</sub>Hf<sub>0.2</sub>W<sub>0.2</sub>C showed the highest melting point of 3495 K. The investigated HECs exhibited exceptional mechanical and thermal stability: hardness: 23 – 36 GPa; elastic modulus: 330– 460

GPa; and melting point: 2761 – 3495 K. Evaluation of mechanical stability from elastic moduli, Poisson's ratio, Cauchy Pressure, and Pugh's ratio suggest that the studied HECs potentially exhibit remarkable resistance to cracks. Fig. 1(a) reveals that the studied ceramics exhibited a linear relationship between fracture toughness and Young's modulus which is otherwise not so true universally. This highlights a well-balanced combination of toughness and rigidity indicating that the studied HECs maintain good resistance to crack propagation without sacrificing stiffness. Fig. 1(b) infers that, the HECs exhibited high Young's modulus (330–465 GPa) while the density was 10,800 - 12,300 kg/m<sup>3</sup>, proposing that HECs are stiffer materials irrespective of density, which makes them promising materials for both lightweight and mechanically strong applications. Fig.1 (c) highlights that the HECs exhibited super hardness, which is higher than that of pure carbides affirming the importance of HECs in the world of advanced materials. Electronic and Magnetic properties were assessed through density of states (DOS) analysis highlighting the effect of bonding characteristics on properties of the material. Therefore, the present study highlights the importance of tuning the composition of individual metals to produce HEC with superior properties.

## **PO-22: Electronic Structure of Creatinine and Hydrated Creatinine: Experimental and DFT Analysis of UV-Visible Spectra**

**Swapnali S. Desai<sup>1,2</sup>, Mayur R. Parate<sup>1</sup>, Aatish S. Daryapurkar<sup>3</sup> and Dilip H. Dagade<sup>2\*</sup>**

<sup>1</sup>*Department of Electronics & Communication Engg. IIIT, Nagpur-441 108*

<sup>2</sup>*Department of Chemistry, Shivaji University, Kolhapur-416 004*

<sup>3</sup>*Department of Basic Sciences. IIIT, Nagpur-441 108*

*Email: dhd\_chem@unishivaji.ac.in*

It is well documented that the creatinine is a key biomarker for thyroid dysfunction as well as kidney and cardiovascular issues, hence the field of creatinine biosensing is rapidly growing. One of the important aspects in the development of biosensor for it is the complete molecular level structural information about creatinine and its hydrated form. The present work reports electronic structure exploration of creatinine and its hydrated form through systematic density functional theory (DFT) investigations for which the dispersion and spin-orbit corrected TD-DFT calculations were made in gas phase as well as in aqueous medium (implicit and hybrid implicit/explicit) and the calculated UV-visible spectra were compared with experimental spectra. This enabled us to explore creatinine water interaction for which type

and alterations in electronic transitions of different types were understood through orbital energies and orbital interaction diagrams. We observe that the DFT predicted spectra agrees well with experimental spectra. Furthermore, the water in the solvation shell can lead to mixing of water-creatinine orbitals causing large alterations in the orbital energies of not only of the creatinine but of the water or water clusters in the solvation shell for which intermolecular hydrogen bonding is the main factor.

### **PO-23: Solvation Behaviour of 1-Methyl-3-propylimidazolium Iodide Ionic Liquid in Aqueous and Aqueous Glycine Solutions**

**Vandana Patel and Sanges P. Zodape\***

*Department of Chemistry, Visvesvaraya National Institute of Technology, Nagpur, Maharashtra 440 010*

*\*E-mail: szodape@chm.vnit.ac.in, sanges02@gmail.com*

In present study, the physicochemical interactions of 1-methyl-3-propylimidazolium iodide i.e. [MPIm][I] in aqueous and aqueous glycine solution were analysed at various temperatures. Volumetric and compressibility parameters such as apparent molar volume of solute ( $V_\phi$ ), limiting apparent molar volume of solute ( $V_\phi^\circ$ ), limiting apparent molar expansivity of solute ( $E_\phi^\circ$ ), thermal expansion coefficient ( $\alpha$ ), hepler's constant ( $\partial V_\phi^\circ/\partial T^2$ ), isentropic compressibility of solution ( $\kappa_s$ ), apparent molar isentropic compressibility of solute ( $K_{s,\phi}$ ), limiting apparent molar isentropic compressibility of solute ( $K_{s,\phi}^\circ$ ), limiting apparent molar volume of transfer ( $\Delta_{tr}V_\phi^\circ$ ), and limiting apparent molar isentropic compressibility of transfer ( $\Delta_{tr}V_\phi^\circ$ ) were measured from experimental density and speed of sound data. The findings shed light on the nature of the interactions between [MPIm][I], water and glycine by showing notable variations in these parameters with temperature and solute concentrations. The study adds to our knowledge of the role of glycine as a co-solute and the behavior of ionic liquids in mixed solvent systems by providing useful information on the structure and dynamic behavior of [MPIm][I] in aqueous media.

### **PO-24: Physicochemical and Thermophysical Studies on Jatropha Oil-Based Fatliquor**

**Aswini Annadurai and Md. Sayem Alam\***

*<sup>1</sup>Advanced Materials Laboratory, Polymer Science & Technology Unit, CSIR-Central Leather Research Institute, Chennai – 600020*

*\*E-mail: sayem.clri@csir.res.in, sayemalam@gmail.com*

The present study explores the chemical modification of Jatropha oil through controlled sulfonation to develop a sustainable fatliquoring

agent for leather processing. The introduction of sulfonic ( $-\text{SO}_3\text{H}$ ) groups significantly enhanced the emulsification ability, hydrophilicity, and compatibility of the modified oil with collagen fibers. The sulfonated Jatropha oil (SJO) was comprehensively characterized by physicochemical parameters such as viscosity, conductivity, particle size, and zeta potential, along with thermal analyses (DSC and TGA). FTIR spectra confirmed the successful incorporation of sulfonic groups while maintaining the triglyceride backbone structure. The SJO exhibited improved thermal stability and better penetration within the leather fiber matrix compared to raw Jatropha oil. SEM micrographs revealed uniform lubrication on the collagen network, correlating with enhanced mechanical strength, abrasion resistance, stitch tear strength, and GSM values. Overall, the findings highlight SJO as a promising eco-friendly alternative to conventional petroleum-based fatliquoring agents, supporting the advancement of green chemistry principles in sustainable leather manufacturing.

## **PO-25: Phosphonium Ionic Liquids: A Safer Electrolyte Choice for High-Performance Supercapacitor**

**P. R. Ghorpade<sup>1</sup>, K. P. Vijayalakshmi<sup>2</sup>, G. K. Sharma<sup>1</sup> and S. S. Terdale<sup>1\*</sup>**

<sup>1</sup>*Department of Chemistry, Savitribai Phule Pune University, Pune-411007*

<sup>2</sup>*Analytical & Spectroscopy Division, Vikram Sarabhai Space Centre (VSSC), ISRO, Trivandrum-695022*

*E-mail: santosh.terdale@unipune.ac.in*

Developing safe and efficient electrolytes is a key challenge in improving the performance of supercapacitors. Conventional organic electrolytes offer high voltage but often suffer from leakage and thermal instability. To overcome these issues, ionic liquids are being explored as alternative electrolytes due to their superior safety, chemical stability, and wide electrochemical window.

This study focuses on the synthesis and characterization of a phosphonium-based ionic liquid, triisobutylmethylphosphonium bis(trifluoromethylsulfonyl)imide [ $\text{P}_{4441}$ ][TFSI], and its application as an electrolyte in supercapacitors. The electrolyte was evaluated in combination with reduced graphene oxide–copper (I) oxide (rGO–Cu, O) nanocomposite electrodes serving as working electrodes. The synthesis involved the careful selection of precursors, optimization of reaction conditions, and purification steps to achieve high purity and yield.

Characterization techniques such as nuclear magnetic resonance (NMR), Fourier-transform infrared (FTIR) spectroscopy, and thermal analysis were employed to confirm the chemical structure, purity, and thermal stability of the synthesized ionic liquid. The electrochemical performance of the resulting supercapacitor systems was investigated using cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS), and the results will be discussed in detail.

### **PO-26: Gamma Radiolysis Enabled Palladium decorated Polypyrrole Nanocomposites for Rapid Room Temperature Ammonia Sensing**

**P. B. Thombre, M. R. Katkar, A. S. Jagdale, S. S. Terdale and G. K. Sharma\***

*Department of Chemistry, Savitribai Phule Pune University, Pune 411007  
E-mail: geeta.sharma@unipune.ac.in*

Room-temperature detection of ammonia ( $\text{NH}_3$ ) is essential for environmental and industrial safety monitoring. Conventional metal oxide sensors require high temperatures, while conducting polymers like polypyrrole (PPy) to enable ambient operation with tunable properties. In this work, a palladium-polypyrrole (Pd-PPy) nanocomposite was synthesized using interfacial polymerization followed by gamma radiolysis, enabling in-situ and uniform reduction of Pd nanoparticles within the PPy matrix. This radiolytic method provides a clean, chemically free synthesis with strong Pd–polymer coupling. FTIR and XRD confirmed Pd incorporation and partial crystallinity (Fig 1), while SEM showed a nanofibrous network with evenly dispersed Pd particles. TGA revealed a 28 % improvement in thermal stability. The Pd-PPy sensor exhibited a maximum 350 % response to 100 ppm  $\text{NH}_3$  with rapid response (1-3 s) and recovery (18-31 s) times, demonstrating stability over multiple cycles. Enhanced charge transfer and catalytic activity from Pd resulted in superior sensitivity and reversibility, making  $\gamma$ -radiolysis derived Pd–PPy nanocomposite as promising material for next-generation room-temperature gas sensors.

### **PO-27: Magnetoelectrodeposition of (Ni-W-Mo) Alloy Coatings for Better Corrosion Protection**

**Shramitha and A. Chitharanjan Hegde\***

*Electrochemistry Research Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, Srinivasanagar -575025, Karnataka  
E-mail: acrhegde@gmail.com*

Ternary alloy coatings of Nickel-tungsten-molybdenum (Ni-W-Mo) of high corrosion resistance were developed under effect of magnetic

field (B), applied parallel to the process of electrodeposition. Magnetic field effect has been used as the tool to alter the crystallinity, composition, and hence corrosion resistance of alloy coatings. Coatings of varying compositions were developed on mild steel at optimal current density by inducing B of varying intensity, in terms of magnitude and direction. It was demonstrated that under optimal conditions, magneto-electrodeposited (MED) Ni-W-Mo alloy coatings are several times more corrosion resistant than its conventional counterpart. Drastic increase in the corrosion resistance of MED (Ni-W-Mo) alloy coatings was attributed to its increased Ni content, affected due to higher paramagnetic property of  $\text{Ni}^{+2}$  ions. The reasons responsible for decreased corrosion rate of MED (Ni-W-Mo) alloy were validated through FESEM, EDX and XRD analyses. Better corrosion resistance of MED (Ni-W-Mo) alloy coatings were explained in the light changed limiting current density ( $i_L$ ) of ions in the bath, due to magnetohydrodynamic (MHD) effect. The inherent limitation of the bath associated with principles of electroplating, inhibited the formation of Ni rich alloy coatings has been successfully alleviated using magnetic field effect. The experimental results are discussed by highlighting benefit of magnetic field effect, in relation to conventional electroplating.

## **PO-28: Optimization of New (Co-V) Alloy Bath for Better Corrosion Protection**

**Nandana N. and A. Chitharanjan Hegde\***

*Electrochemistry Research Laboratory, Department of Chemistry National Institute of Technology Karnataka, Surathkal, Srinivasanagar -575025, Karnataka  
E-mail: acrhegde@gmail.com*

Binary alloy coatings of cobalt and vanadium represented as (Co-V) has been electrodeposited from aqueous acidic citrate bath on mild steel, using sulphamic acid as the brightener. Deposition parameters and bath compositions were optimized using the Hull cell method. Bright and uniform (Co-V) alloy coatings were developed at different current density ( $1.0 - 6.0 \text{ A dm}^{-2}$ ), and their corrosion performances were evaluated by electrochemical AC and DC methods. Experimental results revealed that corrosion resistance of (Co-V) alloy coatings increased with current density up to  $5.0 \text{ Adm}^{-2}$  and then started decreasing. Experimental results showed a linear increase of corrosion resistance of Co-V alloy coatings with current density, attributed to its increased Co content, while its V is decreased. Increase of Co (noble) content with deposition current density indicated that the bath follows anomalous type co-deposition. X-ray diffraction (XRD) confirmed the formation of a single-phase solid solution of Co and V across all current densities. The influence of bath chemistry and

current density on composition, morphology and corrosion performance of alloy coatings are studied, and results are discussed.

## **PO-29: Development of Sustainable Heterogeneous Catalysts for Energy and Environmental Applications**

**Venkata Krishnan**

*School of Chemical Sciences, Indian Institute of Technology Mandi, Himachal Pradesh*

*E-mail: vkn@iitmandi.ac.in*

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. Our research group has recently developed several two-dimensional materials supported on nanostructured photocatalysts 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, our group has also utilized these materials for plastics upcycling, carbon dioxide conversion and Green organic transformations, either by functionalization or doping with a heteroatom. The highlights of the ongoing research work of our group in sustainable chemistry and heterogeneous catalysis will be presented.

## **PO-30: Capturing Carbon with Precision: The Evolving Role of MOFs in CO<sub>2</sub> Mitigation.**

**Saloni<sup>1</sup>\* and Rohit Kumar Rana<sup>2</sup>**

*<sup>1</sup>Department of Chemistry, School of Basic Sciences, Central University of Haryana, Mahendergarh-123029*

*<sup>2</sup>Department of Polymer and Functional Materials, CSIR-IICT, Hyderabad  
E-mail: salonimoudgil7@gmail.com*

This study investigates the synthesis, modification, and characterization of HKUST-type MOFs for enhanced CO<sub>2</sub> capture. Cu-HKUST was systematically doped with Fe<sup>3+</sup> and Gd<sup>3+</sup> to tailor porosity, surface chemistry, and adsorption behaviour. Among all samples, 5% Gd-doped HKUST exhibited the highest uptake (3.7 mmol g<sup>-1</sup>), attributed to defect generation and improved Lewis acidity. Structural analysis confirmed successful metal incorporation, while BET and adsorption studies highlighted significant performance enhancement at optimal doping levels. These findings demonstrate the potential of controlled rare-earth incorporation in developing next-generation MOFs for efficient and sustainable CO<sub>2</sub> capture.



## PP-CYSA-01: Cyclic Ammonium Halides-Based Ionic Liquids for Better CO<sub>2</sub> Absorption and Regeneration

K. Devaiah and Ramesh. L. Gardas\*

*Department of Chemistry, IIT Madras-600036*

*\*E-mail: gardas@iitm.ac.in*

The alarming rise in the atmospheric temperature is primarily due to emissions of greenhouse gases into the atmosphere. Among these emitting gases, CO<sub>2</sub> is one of the gases that can hold more heat than its molecular weight because this gas is acidic in nature. To address this challenge, CO<sub>2</sub> capture is a way to absorb the CO<sub>2</sub> from the atmosphere, and it helps to reduce emissions in the atmosphere. To absorb CO<sub>2</sub>, a solvent medium is required. Thanks to Ionic Liquids (ILs), which have exceptional physicochemical properties, to help with better CO<sub>2</sub> absorption. Among the ILs, Halides containing cyclic amines have better absorption capacity and regeneration capacity than the alkanol amines and acyclic amines. In this study, we present the novel cyclic ammonium halides based ILs, which are synthesized from morpholine, piperidine, and haloalcohols. The synthesized ILs have shown better CO<sub>2</sub> absorption capacity and regeneration, and along with these, they have less viscosity, more free volume, and higher ionic conductivity. Furthermore, these ILs tend to form Deep eutectic solvents (DESs) because of their low melting points. These cyclic ammonium halides have multifunctional Characteristics, which can form versatile solvents with exceptional outcomes for CO<sub>2</sub> capture.

## PP-CYSA-02: Investigation of $\beta$ -diketone based Deep Eutectic Solvents for Lithium Recovery Applications

Zayana S. Nazar and Ramesh L. Gardas

*Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036*

*E-mail: gardas@iitm.ac.in*

Lithium is a critical metal widely utilized in lithium-ion batteries, photovoltaic devices, ceramics, and metallurgical processes. With the rapid growth of energy storage technologies, the demand for lithium continues to increase, necessitating efficient extraction and recovery strategies from various resources. Liquid–liquid extraction using deep eutectic solvents (DESs) has gained significant attention due to their green nature, operational simplicity, low volatility, tuneable selectivity, and potential reusability. DESs are formed by combining a hydrogen bond donor (HBD) and a hydrogen bond acceptor (HBA), generating strong intermolecular interactions that lead to a deep depression in melting point relative to the parent components. Previous studies indicate that  $\beta$ -diketone-based systems can bind lithium ions through chelation, leading to improved selectivity and extraction performance.

In this work,  $\beta$ -diketone-based mixtures are explored at different molar ratios to evaluate their phase behaviour and potential applicability for lithium extraction from aqueous media. Preliminary observations and characterization studies aim to establish suitable combinations capable of functioning as efficient DESs, thereby contributing to the development of improved solvent systems for sustainable lithium recovery.

### **PP-CYSA-03: Fe-Doped Activated Carbon Derived from Dragan Fruit Peel for the Trace-Level Detection of 4-CPAA in Environmental Samples**

**Deepa Jadhav, S. Dhanalakshmi, M. Sreenivasulu and Nagaraj P. Shetti\***

*Centre for Energy and Environment, School of Advanced Sciences, KLE Technological University, Hubballi-580031, Karnataka  
E-mail: npshetti@kletech.ac.in*

Carbon paste electrodes (CPEs) are widely used in electroanalytical applications due to their chemical stability, broad electrochemical window, low capacitive current, ease of fabrication, and renewable surface. Incorporating electrocatalysts into CPEs further enhances their versatility. Inefficient biowaste management in agriculture, driven by high moisture content and low biological stability, accelerates microbial degradation, attracting pests and contributing to greenhouse gas emissions. As such, organic waste offers a valuable resource for electrocatalyst development. Activated carbon (AC), known for its high conductivity and porous architecture, has demonstrated excellent performance in electrochemical applications by promoting efficient electrocatalysis. In this study, AC derived from dragon fruit peels is utilised as a sensing material for the electrochemical detection of the synthetic compound 4-chlorophenoxyacetic acid (4-CPAA). The material was characterised using SEM, FT-IR, XRD, EDX, CV, and EIS, confirming favourable morphological, structural, and electrochemical properties, including enhanced charge transfer. The fabricated sensor exhibits a low detection limit, good linearity, and high recovery rates, even in the presence of common interferents.

### **PP-CYSA-04: S-doped Activated Carbon Derived from Banana Peel for Trace-level Detection of Thymol in Spiked Water, Soil, and Vegetable Samples**

**Shweta Baliger, M. Sreenivasulu and Nagaraj P. Shetti\***

*Center for Energy and Environment, School of Advanced Sciences, KLE Technological University, Hubballi-580031, Karnataka  
E-mail: npshetti@kletech.ac.in*

Thymol (THY), a naturally occurring monoterpenoid phenol found in thyme and related plants, is commonly used in pesticides for its

antibacterial and antifungal properties. Although less toxic than synthetic variants, excessive or improper use can negatively affect human health, aquatic organisms, and the environment. In the current study, we established a simple, profitable, and highly sensitive electrochemical sensor for THY detection in water and soil, utilizing sulfur-doped activated carbon derived from banana peel biowaste. These activated carbons offer advantages such as low cost, enormous surface area, hierarchical porosity, and oxygenated functional groups, making them suitable for various sensing applications. The synthesized material was characterized via SEM, FT-IR, XRD, EDX, AFM, CV, and EIS, revealing optimized morphology, functional surface properties, and efficient charge transfer. The S-BAC600/CPE electrode exhibited a low detection limit of  $0.682 \times 10^{-8}$  M, good linearity, and retained 98-99% of its initial performance after 20 days of storage. Recovery studies using spiked vegetable, fruit, water, and soil samples yielded the values between 86.0% and 95.9%, with RSDs from 1.29% to 2.89%, confirming the sensor's robustness, stability, and practical utility.

### **PP-CYSA-05: Synthesis and Characterizations of Titanium Dioxide Nanoparticles: A Multidisciplinary Approach for Welfare of Society**

**Nandkishor B. Shirsath and Tulsidas S. Savale**

*Department of Chemistry, MGVS M.S.G. Arts, Science, and Commerce College, Malegaon, Savitribai Phule Pune University, Pune (MH)  
E-mail: shirsathnandkishor91@gmail.com*

The present study describes the development of a nano-TiO<sub>2</sub> based composite of starch-co-poly(acrylamide) copolymer. The graft copolymer was characterized by Fourier transform infrared (FT-IR), thermal gravimetric analysis (TGA), scanning electron microscopy (FE-SEM), and X-Ray Diffraction (XRD) confirmed that acrylamide (AM) was grafted onto starch successfully. The effects of pH, initiator dosage, temperature, and time on grafting percentage (GP) and grafting efficiency (GE) were also investigated. The synthesized TiO<sub>2</sub> nanoparticles have successfully enhanced the thermal and biological properties of a native copolymer which was confirmed by TGA and biological assay. This synthesized nanocomposite starch-co-poly (acrylamide) was used as a superabsorbent polymer (SAP) with great thermal property and antibacterial activity which regulates the growth of the plant. With this synthesized nano-TiO<sub>2</sub> of can employed in society to control mosquito larvae which show very good ant larvicidal activity against the material vector.

## **PP-CYSA-06: Scattering-Dependent Thermoelectric Behavior of Wurtzite PbTe: A Numerical Investigation**

**Akshata P. Naragatti and S.B. Kolavekar<sup>1\*</sup>**

*Department of Physics, KLE Technological University, B.V.B.C.E.T Campus, Hubballi, Karnataka 580031*

*E-mail : sangeeta\_k@kletech.ac.in*

In this work, we present a detailed investigation of the thermoelectric properties of the wurtzite (WZ) phase of PbTe by solving the Boltzmann transport equation within the relaxation-time approximation. The electrical conductivity, thermopower, and electronic thermal conductivity are computed by incorporating electron scattering from acoustic phonons and charged impurities. Our results show that the WZ phase of PbTe exhibits extremely low electronic thermal conductivity, reaching 364.11 W/m·K at 1200 K, along with a relatively high thermopower. The calculated thermoelectric figure of merit (ZT) exceeds unity at elevated temperatures, highlighting the potential of WZ-PbTe as a possible promising material at high temperature thermoelectric applications.

## **PP-CYSA-07: Iodide-Induced Fluorescence Enhancement in Polycyclic Aromatic Hydrocarbon-attached Poly Aryl Ether Dendrons: Unusual Emission Response in THF**

**Celin Rooth and Edamana Prasad<sup>\*</sup>**

*Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036*

*E-mail: pre@iitm.ac.in*

Iodide, owing to its inherent heavy atom effect, facilitates intersystem crossing and promotes non-radiative decay, making it a well-established quencher of excited-state emission. This quenching behaviour of iodide has been widely exploited in fluorescence-based sensing strategies, primarily through turn-off mechanisms. However, such approaches often suffer from several limitations. There are a very few reports that have achieved the emission enhancement in presence of iodide, either with the aid of an additional agent or using iodide alone, but only in aqueous media. Here, we present a strategy to enhance the fluorescence of polycyclic aromatic hydrocarbon attached to the poly aryl ether dendron through acyl hydrazone linkage even if it is weakly emissive using iodide alone in THF as the solvent. A detailed mechanistic investigation was carried out to elucidate the origin of fluorescence enhancement observed upon the addition of the well-known quencher iodide to a weakly emissive system in THF.

Spectroscopic and photophysical analyses revealed that iodide interacts noncovalently with the acyl hydrazone linkage of the molecule, leading to the suppression of E-Z isomerism characteristic property of acyl hydrazones. This restriction of molecular motion and the orbital reorientation induced by iodide is proposed to be a key factor contributing to the observed fluorescence enhancement.

### **PP-01: Electrochemical Determination of Mefenamic Acid Using a WO<sub>3</sub>/CTAB/Carbon Composite Electrode**

**Shweta J. Malode and Nagaraj P. Shetti\***

*Center for Energy and Environment, School of Advanced Sciences, KLE Technological University, Vidyannagar, Hubballi-580031, Karnataka  
E-mail: shweta.malode@kletech.ac.in, dr.npshetti@gmail.com*

The electrochemical behavior of an anti-inflammatory drug mefenamic acid (MFA) was studied using a tungsten trioxide (WO<sub>3</sub>) nanostructure-modified carbon paste electrode (CPE) in the presence of a cationic surfactant Cetyltrimethylammonium bromide (CTAB). A significant improvement in the oxidation peak current of MFA was observed at the WO<sub>3</sub>/CTAB/CPE compared to bare CPE. The scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) were employed to evaluate the crystallinity, morphology, and structural properties of the synthesized WO<sub>3</sub>. The electrokinetic parameters, including the effects of temperature, heterogeneous rate constant, scan rate, accumulation time, activation energy, pH, thermodynamic parameters, and the number of protons and electrons involved in MFA electro-oxidation were studied. The fabricated WO<sub>3</sub>/CTAB/CPE with enhanced surface area, stability, and sensitivity detects MFA in pharmaceutical and biological samples, achieving excellent recovery rates.

### **PP-02: Development of Polyelectrolyte Complex Based Silver Nanocomposite Matrix Material for Dual- Drug Delivery in Cancer Treatment**

**Rakshitha and Vishalakshi Badalamoole\***

*Department of Post-Graduate Studies & Research in Chemistry, Mangalore University, Mangalagangothri-574199, Karnataka  
E-mail: rakshitha039@gmail.com, vishalakshi@mangaloreuniversity.ac.in*

Combination chemotherapy is a relatively recent and preferred method in cancer treatment. The delivery of dual drugs in a controlled manner can be achieved with a suitable matrix. In the present work, a polyelectrolyte complex (PEC) of trimethylchitosan and carboxymethyl gum arabic containing silver nanoparticles (SNPs) has been developed as a matrix material for co-delivery of two drugs, 5-

Fluorouracil (5-Fu) and Doxorubicin (Dox). The experimental methods adapted for the modification of chitosan and gum arabic and the formation of PEC nanocomposite have been described. FTIR, FE-SEM, P-XRD, HR-TEM, EDS techniques and zeta potential measurements have been employed in the physico-chemical characterization of the developed nanocomposite material. The presence of SNps with average diameter of 25 nm affected the surface structure and hydrophilicity of the PEC. The swelling study indicated pH responsive nature of the material with higher swelling in simulated intestinal pH conditions compared to simulated stomach pH conditions at pH 7.4 than at pH 1.2. The two drugs, 5-Fu and Dox, were successfully entrapped and subsequently released from the nanocomposite in a sustained manner, aligning with swelling data. Cytotoxicity studies performed with MCF-10A cell lines confirmed the cell compatibility of the nanocomposite and with MCF-7 cell lines indicated the synergistic effect of the two drugs in controlling the cancer cell growth. Thus, the present study demonstrated the potential of the PEC nanocomposite made from modified chitosan and gum arabic as a dual-drug delivery system for cancer therapy.

### **PP-03: Electrochemical Detection of Theophylline using Novel Modified Sensor Graphene Loaded Nano Clay Hybrid Electrode**

**L.S. Killedar and N.P. Shetti<sup>1\*</sup>**

<sup>1</sup>*Department of Chemistry, K.L.E. J. T. College, Gadag. 582102, Karnataka*

<sup>1\*</sup>*Department of Chemistry, School of Advanced Sciences, KLE Technological University, Vidyanagar, Hubballi, 580 031, Karnataka*

*E-mail: dr.npshetti@gmail.com*

Electro-analytical methods are used to quantify the biologically active molecules such as Theophylline (THP) is one of the phosphodiesterase inhibiting drug used in the treatment of asthmatic disorders. High dosage implements some adverse effect on the health. Thus, in the present study we have prepared the electrode by drop casting graphene oxide – nano clay matrix on the glassy carbon electrode surface (GO-NC/GCE), for the quantification of THP. The electrochemical study of THP was done by using cyclic voltammetry and square wave voltammetry techniques. Voltammograms reveals that, higher electro-oxidation peak current of THP at modified electrode suggesting the effective modification of the electrode. From the pH study, it's found that the THP undergone oxidation mechanism involving same number of electrons and protons. The sweep rate effect revealed that, two number of electrons were involved in the diffusion-controlled electrode mechanism. The wide range of linearity was found for GO-NC/GCE,  $3.0 \times 10^{-8} - 5.0 \times 10^{-4}$ M with LOD value



$3.12 \times 10^{-9}$  M. Excipients and Metal ion interference study shows the selectivity and analysis of THP in pharmaceutical drug and spiked urine samples gives the real time applications of modified electrode. We have discovered that modified electrode shows remarkable detection and good recovery value.

#### **PP-04: Synthesis and Characterization of $\text{Cu}_2\text{V}_2\text{O}_7$ Nanoparticles and Evaluation of Corrosion Inhibition Property of Zn- $\text{Cu}_2\text{V}_2\text{O}_7$ Composite Coatings on Mild Steel in 3.5% NaCl**

**J. Chaithra and Y. Arthoba Nayaka\***

*Department of Chemistry, School of Chemical Sciences, Kuvempu University, Shankaragatta- 577 451*

*\*E-mail: drarthoba@gmail.com, chaithraj017@gmail.com*

The current study focused on the synthesis of  $\text{Cu}_2\text{V}_2\text{O}_7$  nanoparticles through a simple co-precipitation method, with analyses performed using various techniques including XRD, FESEM, EDX, UV-Visible spectra and FTIR. The synthesized nanoparticles were subsequently employed for co-deposition with zinc matrix onto mild steel using the electroplating technique, and further analyses were conducted using FESEM, EDX, FTIR, and contact angle measurements. Electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization studies were conducted to evaluate the corrosion inhibition properties of the Zn-  $\text{Cu}_2\text{V}_2\text{O}_7$  composite coating on mild steel in a 3.5% NaCl solution. It was observed that the inclusion of nanoparticles into the zinc matrices improves the corrosion resistance of mild steel.

#### **PP-05: Thermodynamic Properties and FTIR Studies of a Binary Liquid Mixture of N, N-Dimethylacetamide with Water at Different Temperatures**

**Rolee Verma and Ranjan Dey**

*Thermophysical Properties Lab, Department of Chemistry, Birla Institute of Technology and Science, Sancoale, Goa, 403726*

*E-mail: p20230015@goa.bits-pilani.ac.in*

Industrial solvents are used for dissolving, extracting, drug delivery of other chemicals without any chemical change in either solvents or treated substance. It is found in different kind of product such as cleaners, degreasers, paints, cosmetics etc. The thermophysical properties of N, N-Dimethylacetamide (DMAc) and water mixtures play a significant role in industrial applications like polymer processing, pharmaceuticals, nanomaterials, and biochemical systems. In the present investigation, molecular interaction studies have been carried out using the thermophysical properties and FTIR spectroscopy for



the binary mixture of N, N-Dimethylacetamide (DMAc), and water. Experimentally, density ( $\rho$ ) and ultrasonic velocity ( $u$ ) have been measured for different concentrations of DMAc- water at different temperatures. Using the experimental data, various parameters have been evaluated such as Excess molar volume ( $V_m^E$ ), Excess coefficient of thermal expansion, Excess Isentropic compressibility ( $\alpha_p^E$ ) and Deviation in ultrasonic speed ( $\beta_s^E$ ). These parameters have been used to interpret the order of intermolecular interaction at varying concentrations of DMAc-water mixture. The obtained results indicate the presence of strong intermolecular interaction between the carbonyl group of DMAc and the hydroxyl group of water, as well as molecular association which is a function of DMAc concentration in water.

### **PP-06: Thermophysical Studies of Ternary mixture of Industrial Solvents with Water**

**Eshita Kakodkar and Ranjan Dey**

*Thermophysical properties Lab, Department of Chemistry, BITS Pilani K K*

*Birla Goa Campus, Goa 403726*

*E-mail: p20240010@goa.bits-pilani.ac.in*

Estimation of thermophysical properties of a ternary mixture consisting of industrial solvents such as dimethyl sulfoxide (DMSO) and N-methyl-2-pyrrolidone (NMP) with water are important for understanding their physico-chemical behavior in various industrial and scientific applications. These solvents exhibit broad solvation capacity, strong polarity, and are widely employed in multifaceted uses such as chemical synthesis, pharmaceutical formulations, and biotechnological applications. In the present investigation, experimental determination of density and ultrasonic velocity have been carried out over the entire mole fraction range at varying temperatures (293.15 K-318.15 K). The excess molar volumes ( $V_m^E$ ) along with coefficient of thermal expansion ( $\alpha_p$ ), isothermal compressibilities ( $\beta_s$ ) and their excess counterparts have been evaluated at all temperatures over the entire mole fraction range which provide crucial information about the interactions occurring between the components. A comprehensive understanding of the thermophysical properties and the nature of these intermolecular interactions is essential for the effective use of the ternary mixture for various processes and to develop their sustainable and greener alternatives for multivarious applications, including drug delivery systems, solvent recovery processes, etc. while enhancing the efficiency, safety, and performance in practical implementations.

## **PP-07: Tailoring the Functionalities of PVA/PVP Biocomposite Films Integrated with Hesperidin to Confer Wound Healing**

**Oshin Jacintha D'souza and Ravindra B. Chougale\***

*P. G. Department of Studies in Chemistry, Karnatak University, Dharwad-580 003  
E-mail: Oshinjacintha@gmail.com*

Recently, increased resistance to synthetic drugs by patients has attracted the researcher's interest in naturally occurring compound-based treatments for wound healing. Among them, bioflavonoids are prominently known for wound healing and have been implemented as an effective strategy in different formulations of wound dressings. Thus, the present work intended to develop wound-healing biocomposite films based on a Poly(vinyl alcohol)/Poly(vinylpyrrolidone) (PP) blend integrated with different amounts of Hesperidin (PPH) and characterized by microstructure, and mechanical study. The fabricated film depicted uniform morphology and enhanced mechanical property at lower concentration of hesperidin. The in-vitro studies revealed that the developed PPH composites enhanced anti-bacterial activity with increasing hesperidin load. Furthermore, improved biocompatibility with accelerated cell proliferation and wound closure efficacy in 24 h for fibroblast cell line was observed. Hence, our cumulative results strongly supported the potential applicability of the PPH biocomposite film as a perfect material to achieve wound healing.

## **PP-08: Electrochemical Behaviour of Ppy-Fe<sub>2</sub>O<sub>3</sub> Nanocomposites on a Modified GC Electrode for the Quick and Real-Time Measurement of Citric Acid**

**Deepali R. Surase, Shamli D. Nikam, S.T. Gaikwad and Anjali S. Rajbhoj**

*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University  
Chha. Sambhajinagar, Aurangabad*

The fabrication of an electrochemical sensor based on polypyrrole-iron oxide (PPy-Fe, Of ) nanocomposites (NC) immobilized on a glassy carbon electrode (GCE) for the quick and real-time measurement of citric acid is studied to evaluate a highly accurate biosensor for detecting citric acid. The Ppy-Fe<sub>2</sub>O<sub>3</sub> synthesized nanocomposites are then characterized using FE-SEM, HR-TEM, FT-IR, XRD and XPS methods to understand their size, structure, and functional groups. A sensor is developed by utilising a bare GCE and Ppy-Fe, Of -NC-GCE modified electrode that identifies citric acid. Using voltammetry, we measure square wave voltammetry (SWV), cyclic voltammetry (CV),

and differential pulse voltammetry (DPV). The observed cyclic voltammetry, differential pulse voltammetry and square wave voltammetry gives response linearly on concentration of citric acid in the range of 10-180  $\mu\text{M}$  with correlation coefficients of  $R^2 = 0.9660$ ,  $R^2 = 0.9572$ ,  $R^2 = 0.9424$  and sensitivity  $0.011 \mu\text{A}/\mu\text{M}\cdot\text{cm}^2$ ,  $0.00214 \mu\text{A}/\mu\text{M}\cdot\text{cm}^2$ ,  $0.001825 \mu\text{A}/\mu\text{M}\cdot\text{cm}^2$  respectively. These results indicate the  $\text{Fe}_2\text{O}_3\text{-NC-GCE}$  exhibited excellent platform and can be used for electrochemical determination of citric acid.

### **PP-09: Niobium Oxide-Graphene Oxide Nanocomposite: A New Platform for Electrochemical Sensing of Hydroxychloroquine**

**Shamli D. Nikam, Deepali R. Surase, Anjali S. Rajbhoj and Suresh T. Gaikwad**

*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University  
Chha. Sambhajinagar, Aurangabad*

Niobium oxide ( $\text{Nb}_2\text{O}_5$ ) nanoparticles have been synthesized and doped them with graphene oxide to produce a  $\text{Nb}_2\text{O}_5\text{-GO}$  nanocomposite destined for electrochemical sensing.  $\text{Nb}_2\text{O}_5$  was obtained by a controlled sol-gel method and was subsequently examined with X-ray diffraction (XRD), Fourier-transform infrared (FTIR) spectroscopy, Raman spectroscopy and transmission and scanning electron microscopy to ascertain its crystalline structure, surface morphology, and chemical composition. Nanocomposite of niobium oxide and graphene oxide achieved a marked enhancement in surface area, intrinsic conductivity and corresponding electrochemical reactivity, all of which contribute to improved sensor performance. A glassy carbon electrode (GCE) modified with the  $\text{Nb}_2\text{O}_5\text{-GO}$  nanocomposite was used for the voltammetric determination of hydroxychloroquine, a commonly used as antimalarial and antiviral drug of current therapeutic relevance. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) analyses indicated that the  $\text{Nb}_2\text{O}_5\text{-GO}$  nanocomposite electrode delivers higher sensitivity, diminutive limits of detection and expanded linear dynamic ranges in comparison to both the unmodified GCE and electrodes modified separately with  $\text{Nb}_2\text{O}_5\text{-GO}$  nanocomposite. The performance enhancement is attributed to the concerted redox contribution of  $\text{Nb}_2\text{O}_5$ , coupled with the outstanding electron shuttle ability of the GO matrix. Accordingly, the  $\text{Nb}_2\text{O}_5\text{-GO}$  nanocomposite emerges as a compelling platform for the design of next-generation electrochemical sensors directed at pharmaceutical and biomedical monitoring.

## **PP-10: Electrochemical Determination of Allura Red using Poly Diethyl Carbamazine Modified Sensor**

**B. Mehaboob Basha, Kailash S. Chadchan and Swastika N. Das**

*Department of Chemistry, BLDEA's V.P. Dr. P.G. Halakatti College of Engineering and Technology, Vijayapura, Karnataka  
E-mail: mbashachem@gmail.com*

The development of sensitive and reliable electrochemical sensors for food dye detection is of significant importance due to their potential health hazards. In this study, we report the electrochemical determination of Allura Red using a poly(diethyl carbamazine) modified carbon paste electrode (PDEC-CPE). The modified electrode was fabricated via electropolymerization, providing enhanced sensitivity and stability compared to the bare electrode. The electrochemical behavior of Allura Red was systematically investigated under varying experimental conditions, including analyte concentration, solution pH, and scan rate. The modified electrode exhibited well-defined redox responses with linear dependence on concentration, demonstrating its suitability for quantitative analysis. The detection performance was evaluated, and the sensor displayed a limit of detection (LOD) of 4.2  $\mu\text{M}$ , highlighting its high sensitivity. Additionally, the electrode showed good reproducibility and stability, indicating its potential for practical application in food safety monitoring. Overall, this work establishes PDEC-CPE as a promising platform for the electrochemical sensing of synthetic food colorants, with scope for extension to other azo dyes of regulatory concern.

## **PP-11: Vanillin-L-isoleucine Condensation Product as a Green Brightener for Zn-SnO<sub>2</sub> Composite Coatings on Mild Steel**

**J. Chaithra and Y. Arthoba Nayaka\***

*Department of Chemistry, School of Chemical Sciences, Kuvempu University, Shankaragatta- 577 451*

*\*E-mail: drarthoba@gmail.com, chaithraj017@gmail.com*

A novel vanillin–isoleucine condensation product was synthesized and evaluated as an eco-friendly brightener for electrodeposited Zn–SnO<sub>2</sub> composite coatings on mild steel from a sulphate bath. The synthesized compound, a Schiff base-type derivative, was characterized by FTIR confirming the formation of a conjugated imine structure. Zn–SnO<sub>2</sub> coatings were deposited from a zinc sulphate electrolyte containing dispersed SnO<sub>2</sub> nanoparticles, both with and without the additive. The influence of the vanillin–isoleucine derivative on coating brightness, surface morphology, and corrosion behaviour was systematically investigated. SEM analysis revealed that the additive

produced finer-grained, smoother, and more reflective coatings compared to the additive-free bath, while XRD confirmed enhanced crystallinity and uniform nanoparticle distribution. Electrochemical measurements showed improved corrosion resistance for coatings obtained in the presence of the additive, attributed to the formation of a compact and homogeneous composite layer. Overall, the vanillin–isoleucine condensation product acts as an efficient, biodegradable brightener for Zn–SnO<sub>2</sub> electrodeposition from sulphate baths, offering enhanced aesthetic and protective performance for mild steel substrates.

### **PP-12: Thermoacoustic Investigations of Molecular Interactions in Industrial Solvent Mixtures at Varying Temperatures**

**Praseeda P. Nair and Ranjan Dey**

*Thermophysical properties Lab, Department of Chemistry, BITS Pilani K K Birla Goa Campus, Goa 403726*  
*E-mail: p20230415@goa.bits-pilani.ac.in*

In this study, we explore the intermolecular interactions in binary mixtures of dimethyl sulfoxide (DMSO), N-methyl-2-pyrrolidone (NMP) and water at varying temperatures and mole fractions. The experimental values are utilized to evaluate adiabatic compressibility ( $\beta_s$ ), deviations in ultrasonic velocity ( $\Delta u$ ), acoustic impedance ( $z$ ) and interaction parameter ( $\chi$ ). The results indicate presence of strong composition and temperature dependent trends which in turn indicate significant variations in molecular association and packing efficiency. The adiabatic compressibility profile suggests extensive molecular ordering and interaction. Acoustic impedance and interaction parameter analysis further confirms the enhanced interactions at specific compositions. These findings are intended to deepen the understanding of solvent mixture behaviors.

### **PP-13: Electrochemically Reduced Graphene Oxide Immobilized with an Anionic Surfactant as a Sensor - Temperature-Based Investigation.**

**Madhura H.P.<sup>1</sup>, Ronald Mascarenhas<sup>1</sup>, Shikandar D. Bukkitgar<sup>2</sup> and Nagaraj P. Shetti<sup>2\*</sup>**

<sup>1</sup>*Department of Chemistry, St. Joseph's University, Lalbagh Road, Bengaluru, 560027 Karnataka*

<sup>2</sup>*Centre for Energy and Environment, School of Advanced Sciences, KLE Technological University, Vidyanagar, Hubballi, 580 031, Karnataka*  
*E-mail: npshetti@kletech.ac.in*

Recently, electrochemical investigations have attracted a large group of researchers in the development of sensors. Reduced graphene

oxide, when immobilized with an anionic surfactant SDS, improved the sensitivity of the fabricated electrode. The effect of phosphate buffer solution as a supporting electrolyte in the pH range of 3.0 – 11.4 was investigated, demonstrating a pH-dependent electrochemical reaction. Further, the dependency of electrochemical behavior at different temperatures was investigated, and various physicochemical parameters were calculated. In addition, the scan rate variation studies were used to determine the heterogeneous rate constant and the number of electrons transferred, and the electrode process was found to be adsorption-controlled. The sensor was further applied to monitor pharmaceutical and spiked urine samples with high accuracy.

## **PP-14: Thermophysical Studies of Mixture of Industrial Solvents**

**Keshav Agrawal, Eshita Kakodkar and Ranjan Dey**

*Thermophysical Properties Lab, Department of Chemistry, BITS Pilani K.K.*

*Birla Goa Campus, Goa 403726*

*E-mail: f20221490@goa.bits-pilani.ac.in*

Accurate estimation of thermophysical properties of liquid mixtures is essential due to their widespread applications in diverse industrial processes. Since the macroscopic behavior of mixtures arises from the interactions among their constituent components, understanding these relationships aids in designing greener and more sustainable solvents to replace conventional toxic ones. However, predicting thermodynamic and transport properties such as density, viscosity, and ultrasonic velocity remains challenging, as these parameters are highly dependent on temperature, concentration, and molecular structure, while their experimental determination is both time-consuming and costly. Therefore, this study employs a range of predictive, correlative, empirical, and semi-empirical models to estimate these properties for various binary and multicomponent mixtures of organic liquids, ionic liquids, and environmentally friendly deep eutectic solvents (DES) at different temperatures. Predictive models such as Collision factor Theory and Nomoto (for ultrasonic velocity) and Bingham, Kendall–Monroe, etc., (for viscosity) are utilized, along with correlative models including Tamura–Kurata, Wijk, Grunberg Nissan, Katti–Chaudhri and Hind (for viscosity). The accuracy and reliability of these models are evaluated using the Average Absolute Percentage Deviation (AAPD). Furthermore, an analysis will be performed to identify systematic patterns or trends responsible for deviations between experimental and calculated values, providing deeper insight into the underlying molecular interactions governing the behavior of these solvent systems.

## PP-15: Development of Fe<sub>2</sub>O<sub>3</sub>/RGO Nanocomposite Infused with CTAB Surfactant Modified Glassy Carbon Electrode for Electrochemical Detection of Promethazine Hydrochloride in Real Samples

Amruta Patri<sup>1</sup>, Sharanappa T. Nandibewoor<sup>2</sup> and Ravindra R. Kamble<sup>1\*</sup>

<sup>1</sup>Department of Studies in Chemistry, Karnatak University Dharwad 580003

<sup>2</sup>Department of Chemistry, School of Advanced Sciences, KLE Technological University, Hubballi, 580031 Karnataka

E-mail: amrutapatri123@gmail.com

In this study, we developed a metal oxide-reduced graphene oxide (RGO) nanoparticles-modified glassy carbon electrode (Fe<sub>2</sub>O<sub>3</sub>/RGO/CTAB@GCE) to facilitate a simple, sensitive, and efficient carbon-based sensor for the trace-level detection of an antihistamine drug promethazine hydrochloride (PMH). Fe<sub>2</sub>O<sub>3</sub> and RGO nanocomposites were created by hydrothermal and chemical processes respectively, the synthesised samples were characterised using Fourier-transform infrared spectroscopy, X-ray diffraction, scanning electron microscopy and atomic force microscopy. Electrochemical impedance spectroscopy (EIS) assessed material performance. We used cyclic voltammetry (CV) and square wave voltammetry (SWV) to study the electrochemical behaviour and detection of PMH at the Fe<sub>2</sub>O<sub>3</sub>/RGO/CTAB@GCE. Outstanding catalytic characteristics, a large electroactive surface area, excellent absorptivity, and synergistic electrochemical activity for promethazine oxidation were demonstrated by the Fe<sub>2</sub>O<sub>3</sub>/RGO/CTAB@GCE. To create an electrochemical sensor with excellent performance, the electrolyte pH, Fe<sub>2</sub>O<sub>3</sub>/RGO/CTAB nanocomposite quantity, preconcentration potential (vs. Ag/AgCl), and duration were all tuned. Under ideal circumstances, the suggested sensor showed linear concentration variations between 0.6 nmol L<sup>-1</sup> and 0.01 μmol L<sup>-1</sup>. The limits of detection and quantitation were 0.36 and 1.21 nmol L<sup>-1</sup> respectively. The proposed sensor demonstrated high sensitivity, quick evaluation, outstanding repeatability and reproducibility. This innovative technique was successfully applied to measure PMH in urine and water samples.

## PP-16: Prediction of Thermophysical Properties Using AI/ML Models

Kavya V., Ishita Bansal and Ranjan Dey

Thermophysical properties Lab, Department of Chemistry, BITS Pilani K K Birla Goa Campus, Goa 403726

E-mail: f20221404@goa.bits-pilani.ac.in, f20221408@goa.bits-pilani.ac.in

The prediction of thermophysical properties such as density,



viscosity, and ultrasonic velocity are essential for understanding intermolecular interactions and designing efficient solvent systems. Conventional experimental determination of these properties is often time-consuming and limited to specific temperature or concentration ranges. In this study, machine learning and AI-based models will be explored to predict ultrasonic velocity and related thermophysical parameters of binary solvent mixtures using physicochemical descriptors as input features. Models such as multiple linear regression, random forest, and neural networks will be evaluated and compared based on statistical parameters like  $R^2$  and Average Absolute Percentage Deviation (AAPD). The predictive results will be analyzed to gain insights into the molecular interactions governing the systems. Thus, this approach will provide a faster and more scalable route for estimating thermophysical properties, enabling greener and data-driven material design.

## **PP-17: Designing Sustainable Nanocomposite Membranes for Simultaneous Water Treatment and Resource Recovery Applications**

**Shivani Ashok Raikar, Ashok Maraddi and S. K. Nataraj\***

*Centre for Nano & Material science, Jain Global Campus, Jain University,  
Jakkasandra Post, Ramanagara, Bangalore 562112  
E-mail: shivaniraikar04@gmail.com, sk.nataraj@jainuniversity.ac.in*

This project focuses on the development of a sustainable nanocomposite membrane by synthesizing a Mn-MOF/MoS<sub>2</sub> composite reinforced with a polyethersulfone (PES) polymer matrix. The Mn-MOF/MoS<sub>2</sub> composite was prepared via a solvothermal process using BDC, manganese acetate, DMF, and MoS<sub>2</sub>, followed by washing, drying, and characterization using XRD, FTIR, FESEM, and zeta potential analyses to confirm its structure and phase. The composite was incorporated into a 20% PES solution in NMP, and membranes were fabricated using the phase inversion technique. The prepared membranes were evaluated for water flux, dye rejection efficiency, metal ion removal, and stability under varying operating conditions. Additionally, advanced characterization using AFM and antifouling studies with humic acid, tannic acid, Congo red, and sodium alginate were conducted to assess surface morphology and fouling resistance. The membrane's performance was further tested for pharmaceutical contaminant rejection using paracetamol, ciprofloxacin, and bovine serum albumin (BSA). Results demonstrated excellent flux recovery, antifouling properties, and high rejection efficiency, highlighting the potential of Mn-MOF/MoS<sub>2</sub>-PES nanocomposite membranes for large-scale industrial wastewater treatment. This study provides valuable

insights into the design of sustainable, high-performance membranes for environmental and industrial applications.

### **PP-18: Sustainably Engineered ZIF-67–Cellulose Nanocomposite PES Membrane for Enhanced Anion Selectivity and Size-Based Separation**

**Gagan Deep G., D.S. Aditya and S.K. Nataraj\***

*Centre for Nano & Material Sciences, JAIN University, Jain Global Campus, Bangalore-562112*

The present study demonstrates the fabrication of a ZIF-67-induced arecanut husk cellulose incorporated polyethersulfone (PES) membrane for advanced wastewater treatment applications. The incorporation of arecanut husk-derived cellulose into ZIF-67 metal–organic frameworks (MOFs) effectively enhance the membrane’s porosity, hydrophilicity, and surface charge characteristics. The synergistic interaction between the biopolymer-functionalized MOF and the polymer matrix promotes improved water flux and selective ion transport behaviour. Remarkably, the modified membrane exhibits superior rejection efficiency toward anionic contaminants compared to cationic species, attributed to the enhanced negative surface potential and size-exclusion effect. The structural integration of ZIF-67 with sustainable biomass cellulose offers a novel route for tuning charge- and size-selective separation mechanisms. Morphological and physicochemical analyses confirm the homogeneous dispersion and stability of the nanocomposite within the polymer network. Overall, the developed bio-MOF hybrid membrane presents a sustainable and efficient approach for high-performance wastewater purification and ion-selective separation technologies.

### **PP-19: Dynamic Wettability and Micellization Behavior of Surface-Active Ionic Liquid in Aqueous and Polymeric Media**

**Rajat Sinhmar and Vickramjeet Singh\***

*Department of Chemistry, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar 144027, Punjab*

*\*E-mail: singhvj@nitj.ac.in*

Wettability dynamics of aqueous surface-active ionic liquid (SAIL) 1-tetradecyl-3-methylimidazolium bromide [C<sub>14</sub>mim]Br solutions were studied on the complete wetting glass surface. Dynamics in wetting were studied in terms of contact line mobility, elapsed time, and SAIL concentrations. Distinct and surprising dynamic wetting states such as autophobing, autonomous drop motion, contact line expansion, droplet splitting, and droplet pinning were observed. These wetting regimes depend on the concentrations of SAIL, and the self-propelled

autonomous motion may result from the adsorption of the SAIL molecules, inducing Marangoni stresses. Interfacial properties were further explored in the presence of polymeric co-solutes (PEG-200, PVP). Critical micelle concentration (CMC) values were determined via conductivity, contact angle, and surface tension, along with thermodynamic parameters ( $\Delta H^\circ_m$ ,  $\Delta G^\circ_m$ ,  $\Delta S^\circ_m$ ,  $\alpha$ ). Increase in concentration of PEG-200 lowered CMC of SAIL but increased it with temperature, while PVP increased CMC of SAIL with an increase in cosolute concentration and temperature. The observed wettability and interfacial modifications have potential applications in surface engineering, microfluidics, smart coatings, and self-cleaning processes.

## **PP-20: Wettability Modulation via Adsorption – Driven Transition from Complete Wetting to Superhydrophobicity**

**Navdeep Kaur and Vickram Jeet Singh\***

*Department of Chemistry, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar 144008, Punjab*

*\*E-mail: singhvj@nitj.ac.in (VJS)*

The wettability of the surface is an important factor in managing surface characteristics, particularly for coatings, sensors and biomedical devices. Here, the wettability of glass substrates was altered in a systematic manner from total wetting  $0^\circ$  state to superhydrophobic ( $>150^\circ$ ) state based on reactive wetting of stimuli-based surface modifiers. The surface modifiers (stimuli) are used to improve wettability and assess through contact angle measurements with water and dodecane drop. Basic methyl groups can make a rough surface superhydrophobic, while longer alkyl or fluoroalkyl chains can further enhance this property. However, many fluorinated incorporate alkyl or fluoroalkyl groups to lower surface substances are known for their environmental stability and potential hazards. Because of these issues, we choose to avoid these chemicals and instead focused on safer, more sustainable alternatives. In this research, we adopted a more straightforward and efficient strategy to reduce chemical use while enabling rapid control over wettability. Stimuli used to change the wettability used here is, Cetyltrimethylammonium bromide (CTAB). A relative analysis of Surface tension, contact angle hysteresis, wettability energy and work of adhesion was presented in this work at  $20^\circ\text{C}$  and  $35^\circ\text{C}$ . The results show, conclusively, that the molecular structure of the adsorbed species, the concentration of the solution, and the liquid of interest all play significant roles in the switching of wettability from hydrophilic to hydrophobic. Also, temperature has a noticeable contribution to altered droplet behaviour, presenting responsive wettability. Overall, this work provides a constructively useful interactions of modifying surface

behaviour through molecular adsorption with far-reaching or practical applications in coatings technology and self-cleaning surface development.

### **PP-21: Bifunctional Aluminophosphate Catalysts for Selective CO<sub>2</sub> Hydrogenation: Towards Sustainable Carbon Utilization**

**Ganesh Srinivasan, Thamizharasi Pugazhenthii,  
Purushothaman S. P.<sup>1</sup> and N.R. Sasirekha\***

*Catalysis Laboratory, CAS in Crystallography & Biophysics, University of  
Madras, Guindy Campus, Chennai 600025, Tamil Nadu*

*\*E-mail: nrsasirekha@gmail.com*

CO<sub>2</sub> is one of the major environmental pollutants, over the years due to the ongoing increase in atmospheric greenhouse gas emissions. Scientists are working towards a carbon capture, utilization, and storage process from large point sources. Instead of storage, utilizing CO<sub>2</sub> by converting it into value-added chemicals and feedstocks via several pathways, in that hydrogenation is a promising approach. Catalytic hydrogenation of CO<sub>2</sub> has tremendous scope in converting CO<sub>2</sub> into high-carbon energy sources such as methanol, ethanol, gasoline, and even jet fuels, using a proper selection of catalysts. The most challenging part lies in the activation of CO<sub>2</sub> because of the high energy involved in the highly stable C=O bond. Both homogeneous and heterogeneous catalysts are used as reducing agents. However, heterogeneous catalysts can be tuned to achieve high selectivity towards a specific product. In this work, aluminophosphate (ALPO) material was synthesized by the hydrothermal method. Bimetals were loaded on ALPO by the incipient wetness impregnation method. All the catalysts were characterized by XRD, BET, HR-SEM, FT-IR, and UV-visible DRS to study their physico-chemical properties. The catalysts were tested for catalytic hydrogenation of CO<sub>2</sub> in a fixed-bed reactor. All the products were analyzed by Gas Chromatography using FID and TCD detectors. The parameters such as time, temperature, GHSV, and ratio of CO<sub>2</sub>/H<sub>2</sub>, and loading of active metal were optimized. The catalysts were found to be highly active towards the hydrogenation of CO<sub>2</sub>.

### **PP-22: Evaluating the Stability of FtsZ Protein using Chemical and Mechanical Disrupters**

**Ragini Kumari and Hema Chandra Kotamarthi\***

*Department of Chemistry, IIT Madras, Chennai-600 036*

*E-mail: hchandra@smail.iitm.ac.in*

The process of cell division is fundamental to all life forms. FtsZ (Filamenting temperature-sensitive Z-mutant) is a conserved protein

in all bacterial species and is crucial for cell division. FtsZ polymers assemble into a ring structure called the “Z-ring” at the mid-cell to initiate division<sup>1</sup>. One proposed model of cytokinesis suggests that the bending of FtsZ polymers upon GTP hydrolysis generates the inward constriction force on the cell wall, leading to septum formation<sup>2</sup>. Given the role of FtsZ as a potential force generator, it is essential to understand its response to mechanical stress in order to construct a qualitative model of the constriction mechanism. We aim to determine the mechanical landscape of the FtsZ protein by probing the structural stability and unfolding pathways under physiologically relevant forces. Further, as both catalytic activity and polymer morphology of FtsZ are shown to have species dependence, we aim to compare the mechanical stability of this protein from *Escherichia coli* and *Mycobacterium tuberculosis* (Mtb). We will employ AFM-based single-molecule force spectroscopy to determine these mechanical properties of the full-length protein and decipher the contributions of individual domains. In addition, FtsZ has been validated as a therapeutic target for antibiotic discovery, particularly against Mtb. Inhibition of Z-ring formation induces filamentous morphology, rendering cells more susceptible to lysis and death. In this context, molecular features that act as “chemical disrupters” of FtsZ polymers represent promising pharmacophores. As part of our study, we are testing a hybrid of “Combretastatin” and “Discoipyrrole” as a possible antibiotic.

### **PP-23: Selective Hydrogenation of Lactose using Supported Metal Nanoparticle Catalyst**

**Partha Dutta, Parasuraman Selvam and Ramesh L Gardas\***

<sup>1</sup>*Department of Chemistry, Indian Institute of Technology, Madras, Chennai 600036, Tamil Nadu*

<sup>\*</sup>*E-mail: gardas@iitm.ac.in*

A common natural disaccharide, lactose found as most abundant constituent in mammalian milk, also present as a major component of the whey, the by-product of casein and cheese industries. The value-added products of lactose viz. lactitol, galactitol & sorbitol majorly manufactured via catalytic Hydrogenation of sugars. Selective hydrogenation of the sugars requires supported Metal Nanoparticle catalysts with the option of recyclability. A few well known noble-metals are promising in this regard but the cost subdue the large-scale manufacture. Among remaining option Ni is the most available alternative used in industry. Metal Nano Particles (MNPs) dispersed in a suitable solid matrix reduces its sintering and leaching, thus preserving the efficiency in activity for recyclability purpose. In the

present work ordered mesoporous silica is used as the solid support and the Nickel MNPs prepared by reducing inorganic salt precursor in different solvents. The mesoscopic order and the nickel phase confirmed through Powder XRD, HRTEM, Confocal Raman and BET analysis. The hydrogenation of Lactose done in a high-pressure batch reactor and the product analysed via HPLC using Carbohydrate column. Result showed major conversion to lactitol along with unreacted lactose and hydrogenated forms of the hydrolysed species.

## **PP-24: Volumetric Properties of Amino Acids in Aqueous Protic Ionic Liquid Solutions: Probing Molecular Interactions**

**Jaspreet Kaur and Vickramjeet Singh\***

*Department of Chemistry, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar 144011, Punjab*

*E-mail: singhvj@nitj.ac.in*

The volumetric properties of amino acids (glycine and L-valine) in (0.05 to 0.20) mol·kg<sup>-1</sup> aqueous solution of protic ionic liquids (PIL) viz. (diethylammonium acetate [DEAAc] and ethanolammonium acetate [EAAc]) were investigated at different temperatures. The density and sound velocity of amino acids in water and in aqueous PIL were measured over temperatures, T = (298.15 to 318.15) K and at 0.1 MPa. Apparent molar volume ( $V_{2,\phi}$ ), partial molar volume at infinite dilution ( $V_2^\circ$ ), partial molar volume of transfer at infinite dilution ( $\Delta_t V_2^\circ$ ), partial molar compression at infinite dilution ( $K_{s,2}^\circ$ ), and partial molar isentropic compression of transfer at infinite dilution ( $\Delta_t K_{s,2}^\circ$ ) were determined from measured density/sound velocity data to investigate the nature of interactions present between solute (amino acid) and co-solute (PIL) in water. The transfer volumes for both amino acids in [EAAc] solutions were positive, whereas, positive and negative transfer volumes were observed for L-valine and only negative transfer volumes observed for glycine in presence of [DEAAc]. Positive transfer volumes indicate the dominance of hydrophilic interactions among the ions of PIL and charged functional groups in amino acids.

## **PP-25: Designing Aqueous Biphasic Systems Based on Phosphonium Salt-Derived Deep Eutectic Solvents and Inorganic Salts**

**Vahishta Katrak<sup>1</sup> and Sushma Ijardar<sup>2\*</sup>**

*<sup>1</sup>Department of Chemistry, Veer Narmad South Gujarat University, Surat, Gujarat*

*<sup>2</sup>Research Scholar, Department of Chemistry, Veer Narmad South Gujarat University, Surat 395007*

*E-mail: sijardar@vnsgu.ac.in*

Deep eutectic solvents (DESs) have emerged as a potential class



of environmentally friendly solvents in recent years, representing an important leap ahead in green chemistry research. Aqueous biphasic systems (ABSs) have also received attention as long-term alternatives to classic liquid-liquid extraction (LLE) procedures for biological material separation, purification, and isolation. The inclusion of DESs into ABSs has opened up new avenues for research and industry due to the low cost of their components, ease of synthesis, tunable physicochemical characteristics, and biodegradability of DESs. ABSs comprised of several DESs and inorganic salts were examined at a temperature of 25°C. The DESs were created using alkyl triphenyl phosphonium bromides as hydrogen bond acceptors (HBAs) and glycols as hydrogen bond donors (HBDs). The resulting DES-based ABSs were characterised by constructing binodal curves and modelling them with Merchuk's empirical nonlinear equation. Tie-line data were examined using the Othmer-Tobias and Bancroft equations. The effect of salt type, alkyl chain length of the HBA, and nature of the HBD on the phase-forming ability of the developed ABSs was investigated systematically.

### **PP-26: Self-Healable, Stimuli-Responsive Bio-Ionic Liquid and Sodium Alginate Conjugated Hydrogel with Tunable Injectability and Mechanical Properties for the Treatment of Breast Cancer**

**Chirag Chavda, Raviraj Pansuriya and Naved I. Malek\***

*Ionic Liquids Research Laboratory, Department of Chemistry, Sardar Vallabhbhai National Institute of Technology, Surat-3950*  
*E-mail: navedmalek@chem.svnit.ac.in*

Designing stimuli-responsive drug delivery vehicles with higher drug loading capacity, sustained and targeted release of anti-cancer drugs and able to mitigate the shortcomings of traditional systems is need of hour. Herein, we designed stimuli-responsive, self-healable, and adhesive hydrogel through synergetic interaction between [Cho][Gly] (Choline-Glycine) and sodium alginate (SA). The hydrogel was formed as a result of non-covalent interaction between the components of the mixture forming the fibre kind morphology; confirmed through FTIR/computational analysis and SEM/AFM images. The hydrogel exhibited excellent mechanical strength, self-healing ability, adhesive character and most importantly; adjustable injectability. In vitro biocompatibility of the hydrogel was tested on HaCaT and MCF-7 cells, showing >92 % cell viability after 48 h. When tested for drug-loading capacity, the hydrogel show 1500 times drug loading for the 5-fluorouracil (5-FU) against the SA based hydrogel. In vitro release data indicated that 5-FU have more preference towards



the cancerous cell condition, i.e. acidic pH (>85 %), whereas the drug-loaded hydrogel successfully killed the MCF-7 and HeLa cell with a  $<IC_{50}$ –1.92 mM value. The studied hydrogel paves way towards controlled and sustained delivery of anti-cancer drug for the treatment of breast cancer.

### **PP-27: One-Pot Ultrasonicated Green Synthesis of some Polybasic-Metal Oxide Mediate Nanopartical and its Microbial Activity**

**K. V. Goswami\***

*Department of Chemistry, The HNSB Ltd. Science College, Himatnagar, Gujarat*

*\*E-mail: singhvj@nitj.ac.in*

An eco-friendly one-pot ultrasonic-assisted green synthesis was employed to synthesize a polybasic–metal oxide nanocomposite with particle sizes below 90 nm. Metal oxide nanoparticles were synthesized using a low-cost co-precipitation approach, and the polybasic–metal oxide nanocomposite was formed in situ using an ultrasound, single-step oxidative polymerisation process. This approach promoted a uniform dispersion of the metal oxide nanoparticles inside the polybasic matrix, which improved the physicochemical interactions between the organic and inorganic phases. The structural and morphological properties of the nanocomposite were thoroughly investigated using UV, FTIR, SEM, X-ray diffraction (XRD). Furthermore, the antibacterial activity of the polybasic–metal oxide nanocomposite was tested against *E. coli*, *S. aureus*, and *S. typhi*. The nanocomposite exhibited better antibacterial activity against *E. coli* and *S. aureus* but reduced activity against *S. typhi*. The observed antibacterial behavior was due to the synergistic interaction between the polybasic medium and metal oxide, which resulted in improved disruption of bacterial cell membranes. Overall, polybasic–metal oxide nanocomposite synthesized via this green, one pot ultrasonic assisted synthesis technique showed remarkable multifunctional capabilities, making it a prospective way for applications in antimicrobial materials.

### **PP-28: Multifunctional IL@MOF Composite- Based Hydrogel for Enhanced Transdermal Drug Delivery of 5-Fluorouracil**

**Ishani Pandya and Naved Malek\***

*Ionic Liquids Research Laboratory, Department of Chemistry, Sardar Vallabhbhai National Institute of Technology, Surat-395007, Gujarat*

*E-mail: navedmalek@chem.svnit.ac.in*

Advances in biomaterial-based transdermal drug delivery systems

(TDDS) are unlocking new possibilities for cancer therapy by enhancing skin permeability and enabling sustained drug release while minimizing systemic side effects. In this study, we developed a hydrogel platform by encapsulating varying ratios of ionic liquids (ILs) into the micropores of judiciously selected metal-organic frameworks (MOFs), aiming to improve drug loading and delivery performance. Specifically, we utilized [TMG][OI] IL, UiO-66-NH<sub>2</sub> MOF, and carboxymethyl cellulose sodium salt to fabricate a synergistic composite hydrogel. The resulting system demonstrated outstanding thermal stability, mechanical strength, self-healing properties, and spreadability—key attributes for efficient TDDS applications. Biocompatibility assessments using HaCaT cells showed ~90% cell viability, confirming its cytocompatibility. Composite hydrogels prepared with [TMG][OI]@UiO-66-NH<sub>2</sub> at ratios of 0.1:1 (G1) and 0.25:1 (G2) exhibited high drug-loading capacities of 671 mM and 397.8 mM for 5-fluorouracil (5-FU), respectively. In vitro transdermal drug penetration over 48 hours reached 76.4% for G1 and 82.7% for G2. Furthermore, cytotoxicity studies on A431 and MCF-7 cancer cell lines confirmed the therapeutic potential of the drug-loaded hydrogels. Overall, the biocompatible [TMG][OI]@UiO-66-NH<sub>2</sub>-based hydrogel system offers a promising strategy for the transdermal delivery of hydrophilic anticancer agents, supporting its potential for future clinical translation in cancer therapy.

## PP-29: Role of Bi<sub>2</sub>O<sub>3</sub> in Modulating the Some Elastic Properties of Lithium Borate Glasses

Sangeeta B. Kolavekar<sup>1\*</sup>

*Department of Physics, KLE Technological University, B.V.B.C.E.T Campus, Hubballi, Karnataka 580031*  
*E-mail : sangeeta\_k@kletech.ac.in*

This study examines the elastic properties of borate-based glasses with the composition 35B<sub>2</sub>O<sub>3</sub> + 15Li<sub>2</sub>CO<sub>3</sub> + xBi<sub>2</sub>O<sub>3</sub> + (50-x)PbO (where x ranges from 0 to 50 mol%) using the theoretical Makashima-Mackenzie and Rocherulle models. The influence of substituting Bi<sub>2</sub>O<sub>3</sub> for PbO on the elastic moduli was analyzed. The density and molar volume of the glasses were measured, providing input for the theoretical calculations. The Makashima-Mackenzie model was applied to predict the Young's modulus and shear modulus based on the packing density and dissociation energy of the glass components. The results show that the substitution of Bi<sub>2</sub>O<sub>3</sub> for PbO leads to a notable increase in the predicted elastic moduli, reflecting enhanced rigidity and structural integrity. These variations are discussed in relation to the structural role of Bi<sub>2</sub>O<sub>3</sub> and PbO within the borate network. The findings highlight the potential of these glasses for possible applications

requiring specific mechanical properties, such as in optoelectronic and structural materials.

### **PP-30: Impact of Doping on Optical Characteristics of Thin Films of Diketones Derivatives**

**G.V. Muddapur\***

*Department of Physics, KLE Technological University, B.V.B.C.E.T Campus, Hubballi, Karnataka 580031*

*E-mail: muddapur.gangadhar@gmail.com*

In this research paper, we investigate the impact of doping on the optical characteristics of thin films of diketones derivatives prepared via spin coating method. Specifically, we focus on the newly synthesized diketone derivative DK-2 and its effect on the optical properties of the thin films. The transparent thin films were investigated in the field of photonics applications. Various spectroscopy methods were used to characterize the samples. UV-Vis spectrophotometer was used to produce absorption spectra for DK-2 doped samples. The absorption spectra were used to quantify other important optical parameters such as the refractive index, extinction coefficient, and band gap energies. These parameters were investigated with the effect of doping concentration. Fluorescence spectrophotometers were used to record the emission spectra and described doping effects. FTIR spectra of the thin films were also obtained and compared with pure molecule to detect changes in intensity and peak values. The theoretically calculated band gap was determined using DFT/TDDFT method B3LYP 6-311++ (d, p) basis set and compared with experimental results. The results of this study provide insights into how doping affects the optical properties of thin films of DK-2. The study also highlights the potential use of these samples in photonics application.

### **PP-31: Size Dependent Opto-Electronic Properties of SnSe Nanoparticals**

**Eva Meghana, Shivakumar Mathapati and Rajashree M. Hodlur\***

*Department of Physics, School of Advanced Sciences, KLE Technological University, Hubballi-580031, Karnataka*

*E-mail: rm.hodlur@kletech.ac.in*

This study aims to synthesize and tune the particle size of SnSe nanoparticles using a facile and cost-effective method. Tin(II) chloride dihydrate ( $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ ) and selenium dioxide ( $\text{SeO}_2$ ) were used as precursors for tin and selenium, respectively, with 3-mercaptopropionic acid (3-MPA) as the capping molecule. The precursors were mixed in a 1:1 ratio and heated for two and half hours with a condensation tube attached, with samples extracted at 30-minute intervals. The samples

exhibited a change in color, indicating the formation of SnSe nanoparticles. The XRD analysis confirmed the formation of pure SnSe nanoparticles in two of the samples, matching the JCPDS card no. 01-089-0235. The results demonstrate the successful synthesis of SnSe nanoparticles with controlled particle size, which is crucial for optimizing their opto-electronic properties for various applications. The study provides insights into the synthesis and characterization of SnSe nanoparticles, highlighting the potential for scalable and efficient production of these materials.

# INDEX

## SYMPOSIUM

B		S	
Bose S.	PSIL-04	Sainath A.V.S.	PSIL-03
		Sridhar S.	PSIL-05
G		V	
Gupta V.	PSIL-01		
		Venkatesu P.	PSIL-06
H			
Halgeri A.B.	PSIL-02		

## ANALYTICAL & ENVIRONMENTAL CHEMISTRY SECTION

A			
Abbar J.C.	AEO-9	Altaf S.	AEO-03
	AEO-CYSA-14, AEP-22	Amreen K.	AEP-CYSA-17
Achur R.	AEP-09	Amrutha B.M.	AEP-32
Aditya D.S.	AEO-02,AEP-11,16	Anitha G.	AEP-17
Ahmad A.	AEP-04	Ankitha G.N.	AEP-09
Ahmed K.	AEP-04	Anoushka	AEO-13
Aishwarya K.G.	AEP-CYSA-01	Attar T.S.	AEP-13
Ali B.	AEP-CYSA-17	Ayachit N.H.	AEO-20,AEP-31

<b>B</b>		Gayakwad N.	AEP-30
Babu R.S.S.	AEP-CYSA-09	Ghuge P.	AEO-CYSA-02
Badiger N.M.	AEO-20,AEP-31	Gnanakumar G.	AEO-02
Bagul G.N.	AEP-15	Goel S.	AEO-CYSA-17
Balikai C.	AEO-05		AEP-CYSA-17
Banapurmath N.R.	AEO-20	Gopal B.	AEO-CYSA-18
Banoth N.	AEO-16	Gowda J.I.	AEP-08
Banoth N.K.	AEO-15	<b>H</b>	
Bartaria V.	AEP-CYSA-03	Hegde S.N.	AEO-CYSA-05
Bawa S.	AEO-06	Hemavathi A.B.	AEO-02,AEP-11
Bharath K.S.P.	AEP-CYSA-13	Herrmann H.	AEO-CYSA-09
Bhat S.D.	AEIL-07	Hiremath G.B.	AEP-31
Biswas B.	AEO-16,AEP-21	Hosamani M.M.	AEO-20
Borane T.R.	AEP-15	<b>I</b>	
Bukkitgar S.D.	AEP-12	Ibrahim M.A.	AEO-CYSA-17
<b>C</b>		<b>J</b>	
Chand M.	AEP-10	Jain P.	AEO-01,AEP-07
Chatterjee S.	AEIL-06	Jaksani B.	AEO-15
	AEP-14,AEP-19	Jangid A.	AEP-CYSA-03
Chetana S.	AEP-CYSA-13	Javed A.	AEP-CYSA-17
Chetankumar K.	AEP-06	<b>K</b>	
Choudapur V.H.	AEP-24	Kale S.B.	AEP-16
Chougala N.	AEP-24	Kalkhambkar R.G.	AEO-CYSA-06
<b>D</b>		Kalpana D.	AEO-02
Devaraj S.	AEP-29	Kamble R.R.	AEP-03
Dhanalakshmi S.	AEP-18	Kanaparthi R.K.	AEP-CYSA-09
Dhruthi H.R.	AEO-07	Kanthappa B.	AEP-25
Dubey S.K.	AEP-CYSA-17	Kaushik A.	AEO-CYSA-09
<b>F</b>		Kothiyal N.C.	AEO-06
Fande S.	AEO-CYSA-17	Kulkarni P.R.	AEO-CYSA-14
<b>G</b>		Kulkarni R.M.	AEIL-04
Ganguly A.R.	AEP-CYSA-03	Kumar A.	AEO-04

Kumar A.S.	AEO-CYSA-15	Moulya K.P.	AEO-CYSA-16
	AEP-CYSA-15,16	Muttagi G.A.	AEP-CYSA-12
Kumar D.	AEO-14	<b>N</b>	
Kumar M.R.P.	AEO-19	Naik K.	AEP-28
Kumar R.	AEIL-03,AEP-CYSA-03	Nandibewoor S.T.	AEP-03,28
Kumar S.P.B.	AEO-CYSA-10	Napoleon A.A.	AEP-CYSA-15
Kumar V.	AEO-11,AEP-02	Nataraj S.K.	AEIL-02,AEO-02
Kumara S.B.E.	AEO-CYSA-03		AEP-11,16
Kumara S.B.E.	AEP-06,09	Nayak R.	AEP-CYSA-10
Kumara S.N.	AEP-CYSA-13	Nayak S.R.	AEP-05
Kurundawade S.R.	AEP-28	Nayaka Y.A.	AEP-CYSA-01,07
<b>L</b>		<b>P</b>	
Lande S.R.	AEO-CYSA-12	Pal U.	AEIL-01,AEO-15,16,AEP-21
<b>M</b>		Pardeshi S.K.	AEO-CYSA-02,12
Mahesh R.T.	AEO-8	Pardeshi S.K.	AEP-13
Mallu P.	AEO-CYSA-04,AEP-27	Patil A.S.	AEP-24
Malode S.J.	AEP-18,AEP-CYSA-06	Patil H.A.	AEP-15
Manami R.B.	AEO-CYSA-06	Patil M.B.	AEO-18
Manjunatha J.G.	AEO-CYSA-16	Patil M.R.	AEP-15
	AEP-20,25,26,29,32	Patil P.N.	AEO-20
Manjunatha J.G.	AEP-CYSA-14	Patil S.S.	AEO-10
Manna S.	AEO-12	Paul R.C.	AEP-CYSA-02
Manwaal A.D.	AEP-01	Peter A.E.	AEO-CYSA-09
Marathe Y.V.	AEP-15	Prakash R.	AEP-10
Mascarenhas R.J.	AEO-CYSA-01,11	Priyanka	AEP-14
	AEP-CYSA-02,04,05	Puneeth	AEO-CYSA-03
Matani A.G.	AEO-CYSA-11	Puneeth	AEP-06
Matteppanavar S.	AEP-24	<b>R</b>	
Meena J.	AEP-CYSA-16	Radhika M.	AEP-17
Mehmood S.	AEO-16,AEP-21	Raj V.	AEO-CYSA-04
Mittal N.	AEO-CYSA-07	Rajdeo K.	AEO-17
Mohan D.R.	AEP-14	Rakshith G.N.	AEP-CYSA-13
Mondal D.	AEP-16	Rani M.	AEO-13
Moodi J.I.	AEO-9		



Reddy K.L.	AEP-01	Somya A.	AEO-CYSA-08
Rodrigues P.N.	AEO-CYSA-01	Soni R.K.	AEO-03,AEO-CYSA-07
	AEP-CYSA-02,04,05	Sowmya R.K.	AEP-11
<b>S</b>		Sreenivasulu M.	AEO-CYSA-13
Sahana H.R.	AEP-CYSA-07		AEP-23,AEP-CYSA-12
Sailaja B.B.V.	AEP-05	Sriram D.	AEO-CYSA-17
Sajjan A.M.	AEO-20	Sumanth D.	AEP-26
Sandeep S.	AEP-27	Sumanth G.S.	AEP-06
Sandhya K.	AEO-CYSA-15	Sunith K.K.A.	AEP-CYSA-13
Sanjay G.S.	AEP-27	Swamy B.E.K	AEP-17,AEO-07
Santhakumar K.	AEP-CYSA-16	Swamy N.K.	AEO-CYSA-10
Santhosh A.S.	AEP-27	<b>T</b>	
Santhosh K.N.	AEP-11	Tambe K.	AEO-12,AEO-10
Santosh K.N.	AEP-16	Theertha T.B.S.	AEP-26
Saraf P.C.	AEO-CYSA-02	Timmanagoudar P.L.	AEP-23
Satpati A.K.	AEO-12	Tiwari K.	AEO-01,17,AEP-07
Sawant K.C.	AEP-15	<b>V</b>	
Scholz B.B.M.	AEO-CYSA-09	van Pinxteren M.	AEO-CYSA-09
Senthil K.A.	AEO-CYSA-18	Varshney A.P.	AEO-CYSA-08
Shaikh M.	AEP-04	Venkatrao S.P.	AEO-CYSA-17
Shanker U.	AEO-13	Verma P.	AEO-11
Sharma C.K.	AEP-CYSA-04	Verma R.K.	AEO-04
Sharma V.K.	AEIL-05	Vernekar P.R.	AEP-CYSA-11
Sharmila B.M.	AEP-CYSA-14	Vignesh K.	AEP-CYSA-15
Shetti N.P.	AEIL-08	Vishalakshi B.	AEP-CYSA-10
	AEO-CYSA-05,13	Vishwanath V.	AEO-CYSA-01
	AEP-12,18,23		AEP-CYSA-05
	AEP-CYSA-06,11,12	<b>W</b>	
Shirahatti A.M.	AEO-8	Wadhwa D.	AEP-19
Shirsath N.B.	AEP-CYSA-08	Wali M.S.	AEP-03
Shrivastava V.S.	AEP-15	Warad S.S.	AEP-CYSA-06
Singh B.	AEO-14	<b>Y</b>	
Singh N.	AEO-14	Yadav D.	AEP-02
Singh R.B.	AEP-10	Yesudas Y.K.	AEO-CYSA-18
Singh V.P.	AEP-31		
Singhal R.	AEO-03		

## INORGANIC CHEMISTRY SECTION

<b>A</b>		<b>F</b>	
Ajagekar S.D.	IO-10	Firdaus S.	IO-20
Aswar A.S.	IIL-04	<b>G</b>	
<b>B</b>		Gaikwad S.T.	IO-02
Babar M.D.	IO-CYSA-03	Gaurav H.	IO-20
Banapurmath N.R.	IP-28	Gowda J.I.	IP-11
Bano S.	IO-20	Gudasi K.B.	IO-CYSA-04
Bari A.	IO-20	Gugale G.	IO-21
Bharamagoudar R.C.	IP-25	Gunaga M.P.	IO-11
Bharath K.S.P.	IP-CYSA-03,05	Gupta D.	IO-03
Bhat R.A.	IO-12	Gupta K.	IO-07
Bhovi V.K.	IP-19	Gupta V.K.	IP-18
Bindu B.S.	IP-04	<b>H</b>	
Brahmchari S.	IO-06	Hadrihalli A.	IO-CYSA-02
Bukkitgar S.D.	IP-04,IP-13	Hande S.	IO-21
Butcher R.J.	IO-17	Hegde D.	IO-CYSA-04
<b>C</b>		Hegde G.S.	IP-17
Chandana N.	IP-CYSA-03,-04	Hiremath R.S.	IP-30,31
Chandanshive A.A.	IO-02	Hodlur R.M.	IP-31
Chaudhari H.D.	IO-04,IP-01	<b>I</b>	
Chaudhari J.R.	IP-01	Ikbali M.	IO-23
Chaudhary S.	IO-01	Ilager D.	IP-05,06
Chetana S.	IP-CYSA-05	Indushree V.	IP-CYSA-04
Chikkatti B.S.	IP-28	<b>J</b>	
Choubey A.K.	IO-CYSA-01	Jawale V.	IO-21
Chouhan A.S.	IO-12	Jayswal M.R.	IP-09,10,12
<b>D</b>		<b>K</b>	
Dipake S.S.	IO-02	Kakati S.	IP-29
Darshana V.U.	IP-31	Khushi S.C.N.	IO-CYSA-05

Kim I.S.	IP-03,08	Mishra N.K.	IIL-07
Kociok-Kohn G.	IO-26,IP-12	Mishra N.K.	IP-03,08,IO-08
Kongot M.	IO-11	Mondal D.	IP-16
Korde S.A.	IO-02	Moon P.R.	IIL-03
Koshti P.	IP-25	<b>N</b>	
Kujur J.P.	IIL-03	Nataraj S.K.	IO-22,IP-14,16
Kumar A.	IO-19,26	Nidhi	IO-24,IP-20
	IP-09,10,12,15,27	Ningappa K.S.	IP-CYSA-04
Kumar D.	IO-12	Nipate A.B.	IP-26
Kumar R.	IO-17,23	<b>O</b>	
Kumar V.	IO-14	Omoding D.	IP-10,12
Kumara S.B.E.	IP-23	<b>P</b>	
Kumara S.N.	IP-CYSA-05	Pal S.J.	IO-09
Kumaraswamy N.	IP-CYSA-03	Pardeshi S.K.	IO-CYSA-03,06
Kumari G.	IP-27	Patel H.R.	IP-21
Kumari P.	IIL-05	Pathak D.D.	IIL-03
Kushwaha A.	IO-26,IP-09,10,15	Pathan A.R.	IO-CYSA-03
Kuskur C.M.	IP-23	Patil K.	IO-10
<b>L</b>		Patil M.B.	IP-25
Lal N.	IO-18	Patil S.	IP-28
Lande M.K.	IO-02	Prabhuswamy V.B.	IP-CYSA-04
Langyan R.	IO-01	Prakash O.	IO-07,IP-07,24
Latkar R.V.	IP-16	Prasanna S.B.	IP-CYSA-04
Lekha M.P.	IO-09	<b>R</b>	
<b>M</b>		Rai R.	IP-03
Maiyalagan T.	IIL-06	Rajbhoj A.S.	IO-02
Maraddi A.S.	IO-22,IP-16	Rakshita	IP-05
Mascarenhas R.	IP-04,13	Rakshith G.N.	IP-CYSA-05
Mathad S.	IP-29	Rao M.R.	IIL-08,IP-26
Mathapati S.I.	IP-31	Rathod B.D.	IP-01
Megha M.K.	IP-14	Rendale M.	IP-29
Melinmath S.P.	IP-19	Revankar V.K.	IP-17
Mishra A.P.	IIL-01,IO-03,06	<b>S</b>	
	IO-CYSA-01		



## ORGANIC CHEMISTRY SECTION

<b>A</b>		Chaudhari H.D.	OP-CYSA-01
Achalkumar A.S.	IOL-04		OP-09
Aditya D.S.	OP-15	<b>D</b>	
Ahmed K.	OO-27,OP-03,21,23,24	Das S.N.	OO-05
Akki M.	OO-30	Deepthi P.V.	OP-CYSA-02
Amrutha M.	OP-01	Desai K.R.	IOL-08
Anisha G.L.P.	OO-CYSA-02	Desai S.S.	OO-CYSA-04
Ankith S.	OO-14	Dhananjay	OP-22
Arun M. Isloor	OP-27	Dhanusha K.K.	OP-06
Ashok D.	OO-21	Dnyaneshwar B.K.	OP-14
Aswathi J.	OP-12	Dupade H.	OP-21
<b>B</b>		<b>E</b>	
Balikai V.	OO-CYSA-04	Enumula S.	OP-03
Banu N.H.A.	OP-13	<b>F</b>	
Beneesh P.B.	OP-20	<b>G</b>	
Bhalla V.	IOL-01	Farnood R.	OO-24
Bhat P.M.	OO-23	<b>G</b>	
Bhovi V.K.	OO-03	Gangadhar B.	OP-14
Bodke Y.D.	OP-01	Gaonkar S.L.	OO-18
Bollikolla H.B.	OO-17	Garud D.D.	OO-25
<b>C</b>		Garud D.R.	OP-CYSA-06
Chadchan K.S	OO-05		OP-1618
Channamma M.	OO-11	Ghorai S.K.	OO-14,OO-CYSA-07
Charushil	OO-CYSA-04	Gowdar S.B.	OO-30
Chaturvedi D.	IOL-07	Gupta A.	OO-02,09

Gupta J.	OO-02	Kalluraya B.	IOL-06
<b>H</b>		Kalluraya B.	OP-13
Hapse V.M.	OO-14	Kamat V.	OO-30
Hari K.N.	OO-30	Kamath P.	OO-14
Hegde C.	OP-26	Kamath P.	OO-16
Hegde P.	OO-29	Kamath P.	OO-CYSA-07
<b>I</b>		Kamthe D.C.	OP-16
		Kanade D.	OO-04
Isloor A.M.	OP-CYSA-04	Kanaparthi R.K.	OO-CYSA-02
Isloor A.M.	OP-CYSA-07	Kanaparthi R.K.	OP-22
Isloor A.M.	OO-24,26,31	Katagi K.S.	OP-02
Isloor M.	OO-CYSA-01,05	Katkar V.T.	OP-CYSA-03
Isloora A.M.	OP-CYSA-05	Khan H.A.	OP-24
Ismail A.F.	OP-CYSA-07	Kim I.S.	OP-19
<b>J</b>		Kondhalkar S.S.	OP-CYSA-06
Janardanan D.	OP-12	Krishna A.	OO-06
Jat J.L.	OO-06	Kulkarni P.	OO-12
Jayaprakash H.V.	OO-22	Kumar A.	OP-05
Joseph A.M.	OP-26	Kumar C.S.C.	OO-20
Jyothi K.	OO-29	Kumar P.M.R.	OO-01
<b>K</b>		Kumar R.K.	OO-20
Kadam S.	OO-CYSA-05,06	Kurahatti S.	OO-19
Kademani S.	OP-02	Kurahattia S.	OO-07
Kailas D.	OP-25	Kurhe G.K.	OO-16
Kalbagh M.R.	OO-16	<b>L</b>	
Kalkhambkar R.G.	OO-19	Lagarkha R.	OO-28
Kalkhambkara R.G.	OO-07	Lakshmi B.V.	OO-21

<b>M</b>		Pallot H.	OO-CYSA-01
Mahadik S.S.	OP-16	Panchami H.R.	OP-27
Mahanta N.	OP-10	Pandey N.K.	OP-11
Malladi S.	OO-CYSA-04	Parvatikar P.	OO-05
Manjunath B.N.	OO-CYSA-07	Pasodi P.	OP-CYSA-03
Maraddi A.S.	OO-23	Patel A.	OO-CYSA-03
Martis G.J.	OO-18	Patel H.D.	OO-15
Mathad V.T.	IOL-05	Patel M.P.	OP-09
Melinmath S.P.	OO-03	Patel M.V.	OP-CYSA-01
Mendonca N.R.	OP-CYSA-04	Paymode N.	OO-CYSA-05,06
Mishra N.K.	OO-CYSA-08	Pirzada M.R.	OO-26
	OP-19	Poojary B.	OO-30
Mishra S.K.	OP-04	Prabhakar N.	OP-CYSA-07
Murthy C.B.	OO-22	Prajapati A.J.	OP-CYSA-01,OP-09
<b>N</b>		Prakash R.	OP-11
Nafees S.	OO-CYSA-08	Prasad N.R.	OP-17
Naral D.	OO-29	<b>R</b>	
Nataraj S.K.	OO-23,OP-15	Rajamalli P.	OP-14
Nazeruddin G.M.	OP-17	Ranjith P.B.	OO-03
Nellur U.	OO-CYSA-04	<b>S</b>	
Nerkar K.A.	OP-CYSA-06	Saha S.	OO-16
Nimbale R.	OP-21	Santhosh K.N.	OP-15
<b>O</b>		Sarasija M.	OO-21
Othman M.H.D.	OP-CYSA-07	Sathe V.	OP-21
<b>P</b>		Satishkumar P.	OO-24
Padaki M.	OO-CYSA-04	Saundane A.R.	OP-CYSA-03



Sayana K.V.	OP-28	Tambe P.	OP-24
Shabbir S.F.	OP-25	Tapkir S.R.	OP-16
Shah D.	OP-10	Tewari A.K.	OO-CYSA-03
Shaikh A.	OO-26	Thabaj K.	OO-CYSA-04
Shaikh A.	OP-23	Torane R.C.	OO-25
Shaikh A.	OP-23	<b>V</b>	
Shaikh A.R.	OP-24	Valsaraj V.P.	OP-08
Shaikh A.R.	OP-25	Varala R.	OO-17
Shaikh S.B.	OP-21	Venkatesh M.	OO-31
Shaikh V.S.	OO-26	Vijesh A.M.	OO-13,OP-06,07,08
Shaikh V.S.	OP-17	OP-CYSA-02	
Shaikh Y.I.	OO-26	Viji K.	OP-07
Shaikh Y.I.	OP-17	Vishwanath T.	OP-28
Sharma V.P.	OO-CYSA-03	Vora J.J.	OP-CYSA-01,OP-09
Sheethal	OP-26	Vyas S.P.	OO-08
Shete S.A.	OO-CYSA-07	<b>W</b>	
Shetti V.	OO-31	<b>Y</b>	
Shivarama B.	OP-CYSA-05		
Shrivastava V.S.	OO-04	<b>Y</b>	
Singh R.B.	OP-11		
Sreelekha K.M.	OP-20	Yadav A.	OP-19
Sridharan M.A.	OO-10	Yadav A.K.	OO-06
Swamy M.D.	OO-31	Yelamaggad C.V.	IOL-02, 03

### T

Tambe P.	OP-03
Tambe P.	OP-21

## PHYSICAL CHEMISTRY SECTION

		<b>D</b>	
<b>A</b>		D'souza O.J.	PP-07
Abbar J.	PO-CYSA-07	Dagade D.H.	PO-22
Aditya D.S.	PP-18	Daryapurkar A.S.	PO-22
Agrawal K.	PP-14	Das S.N.	PP-10
Alam M.S.	PO-24	Dash B.R.	PO-CYSA-01
Anisha G.L.P.	PO-CYSA-11	Dayananda B.S.	PO-CYSA-08
Annadurai A.	PO-24	Deep G.G.	PP-18
<b>B</b>		Desai S.S.	PO-22
Babu R.S.S.	PO-07	Devaiah K.	PP-CYSA-01
Badalamoole V.	PP-02	Devika S.R.	PO-11
Baliger S.	PP-CYSA-04	Dey R.	PIL-03,PP-05,06,12,14,16
Banapurmath N.R.	PO-CYSA-03	Dhanalakshmi S.	PP-CYSA-03
Bansal I.	PP-16	Doddamani R.	PO-13
Basha B.M.	PP-10	Dutta P.	PP-23
Bharath K.S.P.	PO-CYSA-06	<b>G</b>	
Bhutani V.	PO-CYSA-10	Gaikwad S.T.	PP-08,09
Brahma S.	PO-12	Gardas R.L.	PO-10,11,12
Bukkitgar S.D.	PP-13		PO-CYSA-01
<b>C</b>			PP-23,PP-CYSA-01,02
Chadchan K.S.	PP-10	Ghorpade P.R.	PO-25
Chaithra J.	PP-04,11	Goswami K.V.	PP-27
Chaudhary R.R.	PIL-05	Gupta B.	PO-14
Chavda C.	PP-26	<b>H</b>	
Pansuriya R.	PP-26	Harshitha A.	PO-CYSA-07
Chetana S.	PO-CYSA-06	Hegde A.C.	PO-27,28
Chetti P.	PO-09	Hodlur R.M.	PP-31
Chikkatti B.S.	PO-CYSA-03	<b>I</b>	
Chougale R.B.	PP-07	Ijardar S.	PP-25
		Indoria S.	PO-16

Ingole S.B.	PO-02	Malode S.J.	PP-01
<b>J</b>		Maraddi A.	PP-17
Jadhav D.	PP-CYSA-03	Mascarenhas R.	PP-13
Jagdale A.S.	PO-26	Mathapati S.	PP-31
<b>K</b>		Meghana E.	PP-31
Kakodkar E.	PP-06,14	Mishra A.K.	PO-CYSA-01
Kamble R.R.	PO-15,PP-15	Muddapur G.V.	PP-30
Kanaparthi R.K.	PO-07	<b>N</b>	
	PO-CYSA-11	N. Chandana	PO-CYSA-04
Kang T.S.	PIL-06	Nair P.P.	PP-12
Kasar V.	PO-18	Nandana N.	PO-28
Katkar M.R.	PO-26	Nandibewoor S.T.	PO-15
Katrak V.	PP-25		PO-CYSA-09,PP-15
Kaur J.	PP-24	Naragatti A.P.	PP-CYSA-06
Kaur N.	PP-20	Nataraj S.K.	PP-17,18
Kavya V.	PP-16	Nayaka Y.A.	PO-08,PP-04,11
Killedar L. S.	PP-03	Nazar Z.S.	PP-CYSA-02
Kolavekar S.B.	PP-29	Nikam S.D.	PP-08,09
	PP-CYSA-06	Ningappa K.S.	PO-CYSA-04
Kotamarthi H.C.	PO-20,PP-22	<b>P</b>	
Kothandaraman R.	PO-CYSA-10	Padhan A.	PO-16,19
Krishna A.	PO-04	Pandya I.	PP-28
Krishnan V.	PIL-08	Parate M.R.	PO-22
Kumar A.	PIL-01	Patel V.	PO-23
Kumar H.	PIL-04	Patri A.	PO-15,PP-15
Kumara S.N.	PO-CYSA-06	Pattanvall A.	PO-16
Kumari K.	PIL-07	Prabhuswamy V.B.	PO-CYSA-04
Kumari R.	PP-22	Prakash R.	PIL-05
<b>M</b>		Prasad E.	PP-CYSA-07
Madhura H.P.	PP-13	Prasad S.	PO-06
Malek N.	PP-28	Prasanna S.B.	PO-CYSA-04
Malek N.I.	PP-26	Pugazhenthith T.	PP-21

Purushothaman P.S.	PP-21	Singh V.	PO-05,16,19
Pushparekha	PO-CYSA-08		PP-19,24
<b>R</b>			
Raikar S.A.	PP-17	Singh V.J.	PP-20
Rajappa S.K.	PO-CYSA-09	Sinhmar R.	PP-19
Rajbhoj A.S.	PP-08,09	Sistla Y.S.	PO-17,21
Rakshith G.N.	PO-CYSA-06	Solanki P.P.	PIL-02
Rakshitha	PP-02		
Ramanujam K.	PO-12	Sreenivasulu M.	PO-CYSA-05
Rana R.K.	PO-30		PP-CYSA-03,04
Rooth C.	PP-CYSA-07	Srinivasan G.	PP-21
<b>S</b>			
Sahana H.R.	PO-08	Suma J.G.	PO-CYSA-09
Sailani R.	PO-14	Sunith Kumar K.A.	PO-CYSA-06
Sajjan A.M.	PO-CYSA-03	Surase D.R.	PP-08,09
Saloni	PO-30	<b>T</b>	
Sarojini B.K.	PO-CYSA-08	Tabassum N.	PO-21
Sasirekha N.R.	PP-21	Talele P.	PO-01
Satpati A.K.	PO-18	Terdale S.S.	PO-25,26
Savale T.S.	PP-CYSA-05	Thombre P.B.	PO-26
Selvam P.	PP-23	<b>V</b>	
Shaibuna M.	PO-10	Vasanth T.	PO-03
Sharadeeshri H.K.	PO-CYSA-05	Veerananje I.	PO-CYSA-04
Sharma G.K.	PO-25,26	Venkata Krishnan	PO-29
Shendage S.	PO-18	Verma R.	PP-05
Shetti N.P.	PP-03	Vijayalakshmi K.P.	PO-25
	PO-CYSA-02,05	<b>Y</b>	
	PP-01,13,PP-CYSA-03,04	Yadav A.K.	PO-04
Shetti R.S.	PO-CYSA-02	Yadav M.	PO-17
Shirsath N.B.	PP-CYSA-05	<b>Z</b>	
Shramitha	PO-27	Zodape S.P.	PO-23
Singh R.B.	PIL-05		

## INDIAN COUNCIL OF CHEMISTS

Indian Council of Chemists (ICC), was founded at Agra on 19th September, 1981 with an initial membership of more than 100 fellows. However, over the past 45 years it has grown in strength and popularity. At present there are more than 1870 Life Fellows and about 8250 annual floating fellows. The membership includes Scientists, Professors, Researchers, Teachers and Scholars from various IITs, CSIR Laboratories, Universities, Colleges, prestigious academic institutions and scientific organizations spread all over the country. The first Annual Conference of ICC was held at **Agra** and subsequent conferences were held and hosted by various universities / institutions throughout the country such as; Kashmir University, **Srinagar**, Karnataka University, **Dharwad**, Gorakhpur University, **Gorakhpur**, Central Fuel Research Institute, **Dhanbad**, Madurai Kamraj University, **Madurai**, Jiwaji University, **Gwalior**, Sri Venkateshwara University, **Tirupati**, Gulbarga University, **Gulbarga**, Goa University, **Goa**, Bihar University, **Muzaffarpur**, Kakatia University, **Warangal**, Jammu University, **Jammu**, The Institute of Science, **Mumbai**, Dr. B.R. Ambedkar University, **Aurangabad**, Mangalore University, **Mangalore**, Madras University, **Chennai**, North Maharashtra University, **Jalgaon**, Kuvempu University, **Shimoga**, Mysore University, **Mysore**, Rani Durgavati University, **Jabalpur**, Indian Institute of Technology, **Roorkee**, KC College, **Mumbai**, Birla Institute of Technology, **Ranchi**, Birla College, **Kalyan**, Dr. H.S. Gour University, **Sagar**, Gurukul Kangari University, **Haridwar**, H.N.G. University, **Patan**, Panjab University, **Chandigarh**, Osmania University, **Hyderabad**, Saurashtra University, **Rajkot**, Karnatak University, **Dharwad**, Indian School of Mines, **Dhanbad**, Uka Tarsadia University Bardoli, **Surat** and **Haribhai V. Desai College, Pune** in association with **College of Engineering, Pune**, School of Chemistry, Andhra University, **Visakhapatnam**, National Institute of Technology Karnataka (NITK) Surathkal, Mangalore, **Karnataka**, Jaipur National University, **Jaipur**, Veer Narmad South Gujarat University, **Surat**, Sahabana University, **Karimnagar**, IBS, Khandari, Dr. Bhimrao Ambedkar University, **Agra**, Department of Pure & Applied Chemistry University of Kota, **Kota (Rajasthan)**, PES's Modern College of Arts, Science and Commerce, **Pune** & **6 International Conferences** at **Bangkok, Kuala Lumpur, Dubai, Tashkent, Bali** and **Paris** were highly successful and well attended.

### OBJECTIVES

- (i) To advance and promote the cause of chemical research & education in the country.
- (ii) To strive for strengthening co-operation on the national level and promoting contacts amongst scientist of the country.
- (iii) To publish such proceedings, journals, transactions and other material as may be considered desirable.
- (iv) To organize symposium, discussions, special lectures, exhibitions and other related activities for a better understanding of chemical research and its applications for the economic, social and industrial progress of the country.
- (v) To under take any or all other acts, matters and things as are conducive to, or incidental to, or necessary for, the above objectives.
- (vi) To work in association with International Societies of Chemistry and to co-operate with other organizations having similar objectives

### JOURNAL OF THE INDIAN COUNCIL OF CHEMISTS

It is a peer reviewed biannual research journal, published by the Indian Council of Chemists since 1984, which is abstracted in the **Chemical Abstracts**, also included in the UGC approved Journals 2019. The topics of Chemistry, covered under the journal include co-ordination chemistry, electro-chemistry, catalysis, reaction kinetics, biotechnology, synthetic organic and inorganic chemistry, organo-metallics, natural products, corrosion, nuclear chemistry, reaction mechanism and all other areas of chemistry of national and industrial importance and significance, which cover recent topics.

Articles accepted for publication in the **J. Ind. Council Chem.** can be Short Communication, Full Length Manuscripts, Review Articles and Book Reviews

### AN APPEAL

There is a growing demand for the publication of quality research work in peer reviewed journals of international standard. This is the main objective of the **J. Ind. Council Chem.**, which has been publishing original, innovative, quality based articles of recent scientific and industrial importance, for the last Thirty Four years. There is a steady increase in the number of manuscripts received by the **J. Ind. Council Chem.** We intend to increase the number of issues each year.

To meet this challenge, the co-operation of its readers, well wishers and authors is solicited through the introduction and subscription of **J. Ind. Council Chem.** in many more Institutions, Universities, Libraries and Colleges. This will enable us to increase its standard, quality, periodicity and circulation. Therefore, we appeal to all, related to Chemistry through education or research in India and abroad to bring **J. Ind. Council Chem.** to everybody's knowledge and encourage subscription in their institutions and libraries.

# INDIAN COUNCIL OF CHEMISTS

## EXECUTIVE COMMITTEE

### Patron

**Dr. Greesh Saxena (U.P.)**

### President

**Prof. R.K. Verma, (Bihar)**

### Vice-Presidents

**Prof. Balakrishana Kalluraya (Karnataka)**

**Prof. C.P. Bhasin (H.P.)**

**Prof. Pradeep K. Sharma (Rajasthan)**

**Prof. A.P. Mishra (M.P.)**

**Prof. S.T. Nandibewoor (Karnataka)**

**Prof. Somasekhara Rao (Nagaland)**

**Prof. S.K. Pardeshi (Maharashtra)**

**Prof. D.D. Pathak (Jharkhand)**

**Prof. K.R. Desai (Gujarat)**

**Prof. N.B. Patel (Gujarat)**

### Secretary

**Prof. Rajesh Dhakarey (U.P.)**

### Jt. Secretaries

**Dr. S.C. Goyal (U.P.)**

**Dr. Vinod Kumar (U.P.)**

### Treasurer

**Prof. Manoj K. Rawat (U.P.)**

### Zonal Secretary

#### *North Zone*

**Prof. D.P. Singh (Haryana)**

#### *South Zone*

**Dr. K.A. Emmanuel (A.P.)**

#### *East Zone*

**Dr. Kalpana Kumari (Bihar)**

#### *West Zone*

**Prof. G.S. Gugale (M.S.)**

#### *Central Zone*

**Prof. Ajay Taneja (U.P.)**

#### *North-East Zone*

**Dr. Dipak Sinha (Nagaland)**

### Members

**Prof. Ali Mohammad, (U.P.)**

**Dr. Parag V. Adhyapak (M.S.)**

**Dr. B.K. Srivastava, (U.P.)**

**Dr. P. Haritha (A.P.)**

**Dr. Bhoopendra Singh, (U.P.)**

**Dr. Ranjit Kumar (U.P.)**

**Prof. B.B.V. Sailaja, (A.P.)**

**Dr. R.K. Agarwal (U.P.)**

**Dr. Chennupati V. Suresh (A.P.)**

**Dr. R.K. Shukla (U.P.)**

**Prof. J.J. Vora (Gujarat)**

**Dr. Sandip P. Vyas (Gujarat)**

**Dr. Kamod Singh Meena (Rajasthan)**

**Prof. S.A. Chimatadar (Karnataka)**

**Dr. Kalpesh Giri V. Goswami (Gujarat)**

**Dr. Vinod K. Shrivastava (M.P.)**

**Prof. Anand K. Aswar (M.S.)**

**Prof. Shivraj (Telangana)**

**Prof. D Ashok (Telangana)**

**Dr. Rakshit Ameta (Rajasthan)**

**Prof. R.R. Jha (Jharkhand)**