

**REPORT ON THE INDIAN ANALYTICAL SCIENCE CONGRESS 2018 ORGANIZED BY INDIAN
SOCIETY OF ANALYTICAL SCIENTISTS & SCHOOL OF CHEMICAL SCIENCES, MAHATMA GANDHI
UNIVERSITY, KOTTAYAM AT KUMARAKOM, KOTTAYAM, KERALA STATE DURING
FEBRUARY 08-10, 2018**

The Indian Analytical Science Congress (IASC-2018) was organized by the Indian Society of Analytical Scientists (ISAS) Kerala Chapter and School of Chemical Sciences Mahatma Gandhi University, Kottayam at Backwater Ripples Resort, Kumarakom, Kerala, India during February 08-10, 2018. The theme of the conference was, "Innovations and Emerging Advances in Analytical Science and Technology". The Main goals of organizing the conference were to evaluate the status of modern analytical science and Technology in India against the global scenario, to suggest future directions and also to establish and renew national collaboration of analytical chemists and educators, in our country. The congress covered almost all the areas of analytical science and technology and painted a broad canvas dreamed about future capabilities for innovations in this field.

Around 80 research papers have been received from academia, R&D institutions and industry. IASC 2018 provided adequate scientific and social environment for scientists to discuss innovations and emerging advances in the area of analytical science and technology. The present conference held at Kumarakom was the latest in the series of IASC series of conferences organized by ISAS and started in 2007 to promote analytical science and technology in India. This conference also provided an excellent opportunity for young Indian researchers, teachers and students, and scientists from all over the country, a forum to meet the experts and representatives of national scientific community and to re-establish links with their peers and colleagues to enable them to initiate new collaborative work.

Dr Kamachi Mudali, Chairman and Chief Executive, Heavy Water Board, Department of Atomic Energy, Mumbai inaugurated the Conference on February 8, 2018 at Backwater Ripples Resort, Kumarakom. In his inaugural speech Dr Kamachi Mudali talked about the importance of analytical science in the production of nuclear materials particularly heavy water. Analytical sciences play an important role in chemical, nuclear and allied energy, pharmaceuticals, food and preservatives, fertilizer, plastic, etc. The market acceptability of these essential products depends solely on their quality. Analytical Chemistry which is one of the oldest branches of chemistry and foundation block for other branches of chemistry plays a vital role in assessing quality of raw materials as well as products. Analytical techniques such as NMR, FTIR, MS, HPLC, GC etc. are well known techniques used for quality control. These techniques play a key role in determining the product quality and isotopic purity of D- labelled

compounds, NMR solvents and deuterium depleted water. So the theme of the congress is very relevant to DAE ,Heavy Water Board and other research and development organizations. He hoped that the conference will give a boost to the Make in India campaign to attain self-sustainability in the field of energy materials and technology.

A souvenir brought out in commemoration of the conference was released by Dr Kamachi Mudali. In the inaugural session ISAS awards were presented to three eminent scientists of our country. ISAS Life time achievement Award 2016 was presented to Dr Ganapathy Ramakrishnan, Chairman- Chromatographic Society of India, Mumbai in recognition of a lifetime of distinguished achievements and outstanding contributions made by him in the field of chromatography and spectroscopy. The second award, viz. ISAS National Award for Excellence in Science and Technology 2016 was presented to Dr R. Srinivas, Chief Scientist , Indian Institute of Chemical Technology, Council of Scientific and Industrial Research (CSIR), Hyderabad 500 007, Telengana State for his outstanding contributions in the field of Mass Spectroscopy .ISAS National Award for Excellence in Science and Technology 2017 was presented to Dr R.Gopalan, Associate Director, ARCI, Chennai for his outstanding contributions in the field of Materials Science & Engineering, particularly in the research area of Energy Materials for various National Mission Programmes

Shri S.K.Malhotra, President-ISAS presided over the function. In his presidential address Shri Malhotra exhorted the participants to explore how we can use analytical science and technology as the driver of future solutions that make our country better, safer and eco-friendly. Dr Daisy Joseph Secretary- ISAS National body and Dr P.P. Chandrachoodan, Member Executive Committee of ISAS offered felicitations. Prof. Suresh Mathew – Co-Chairman of the organizing Committee welcomed the participants. Dr VR Nair, Chairman-Organizing Committee proposed the vote of thanks. Dr G.Ramakrishnan, Dr R.Srinivas and Dr R. Gopalan, the ISAS award winners also spoke on the occasion.

The inaugural session was followed by technical session I. The technical session I was chaired by Dr P.P.Chandrachoodan, Former Programme Officer, BRNS, DAE, Mumbai. The first plenary address of the conference was presented by Dr G.Ramakrishnan , Chairman – Chromatographic Society of India, Mumbai.. The title of his paper was, “The Importance of Chromatographic and Spectroscopic Techniques “. In his talk he presented the importance chromatography and spectroscopic techniques on our day today lives particularly in environmental analysis, food and beverages analysis, pharmaceutical products analysis, forensic sciences & sports doping.

The second plenary talk was delivered by Dr R.Srinivas, Chief Scientist ,CSIR-IICT, Hyderabad In his presentation Dr Srinivas discussed the identification and characterization of degradation products and metabolites of drugs using LC_ESI-MS/MS. . His lecture focused on some of our recent studies on stress stability studies and in vivo metabolic investigation of drug molecules which have been carried out using liquid chromatography-electrospray ionization tandem mass

spectrometry (LC-ESI-MS/MS). In addition, association of lower levels of vitamin D metabolite with diabetes complications, was also discussed. Dr R. Gopalan, Associate Director, ARCI, Chennai delivered the third plenary talk. He talked on advanced structural characterization tools in the field of material science and their role for clean energy applications. Newer energy materials are emerging and are as well more complex from a chemical and structure points of view along with the development of new synthetic strategies, and thus the study of the correlation between their structure and properties requires the application of advanced characterization techniques in order to understand all the key aspects responsible for the materials' performance. A more accurate description of the processes involved in several materials of interest for clean energy applications requires their structural investigation starting from primary tools such as XRD, SEM, TEM, STEM to the highest spatial resolution viz. 3-dimensional atom probe (3DAP) techniques. In his presentation he also covered a few examples of clean energy materials such as Li-ion batteries, thermoelectric, fuel cells, magnets and the advanced structural characterization tools used to characterize them to understand their performance for energy conversion and storage technologies.

Technical session II was started at 09.30Hours on 9th February 2018 and was chaired by Dr KGK Warriar, Former Deputy Director, CSIR-NIIST, Thiruvananthapuram. The first invited talk in the Session was delivered by S. Narasimhan, Asthagiri Herbal Research Foundation, 162 A, Estate second main road, Perungudi Industrial Estate, Perungudi Chennai 600096. The title of his talk was, "Chromatographic Techniques to Overcome the Challenges in Standardization of Herbal products". In his talk he covered the latest advancements in herbal technology and the innumerable challenges encountered while developing a product that could be accepted universally as per the requirement of regulatory bodies in India and abroad. The main focus is on the standardization methods of fixing the specification of herbal formulations based on the guidelines and the requirements of the regulating authorities in promoting herbal formulations. His presentation dealt with application of chromatographic techniques to overcome the challenges in standardizing herbal products. The second talk was delivered by Dr A.P. Jayaraman, former Advisor, Directorate of Purchase and Stores, Department of Atomic Energy, Mumbai. The title of his talk was, "Expanding Horizons of Global Supply Chains and Procurement challenges in Analytical Instruments and Services". In this paper he presented the features of main stream global supply chains of Analytical Instruments and Services and the emerging trends of the source market including the instrument manufacturing industry of China growing at an annualized rate of 9.5% to \$30.4 billion in 2017. He also described the innovative and advanced spend analysis and procurement analytics solutions developed by supply chain managers to solve complex, data-driven problems in procurement of advanced instruments to secure value for money. Dr Deepak Parab from Metrohm India Limited, Chennai was the next speaker. He talked on the applications of ion chromatography in water and food analysis.

According to him modern ion chromatography system can be set up for fully automated analysis of water, food and beverage samples and can be hyphenated with other techniques to provide complete data of various parameters in short time.

The third technical session was chaired by Dr Jose Panakkal, Former Outstanding Scientist, BARC, Tarapur, Maharashtra. The first paper in the Session was presented by Dr Daisy Joseph, Nuclear Physics Division, Bhabha Atomic Research Centre. The title of her talk was, "Chemical shift studies of 3d elements Mn, Cr, Cu and Zn K-edges by XANES (X-ray absorption Near Edge Spectroscopy) using INDUS-2 Synchrotron Radiation at RRCAT, Indore". X-ray absorption edge of metal ion may change to different extent depending upon the chemical environment viz. effective charge, nature of ligands, co-ordination numbers, electronegativity of anions, covalent character of the bonds, surrounded the metal ion, even at the same oxidation state. This change in the absorption energy of the metal ion in its compound from the pure metallic state (zero oxidation state) is known as the chemical shift ΔE (eV) of the metallic ion. In the present study by means of synchrotron based X-ray absorption spectroscopy study we have calculated the chemical shift and their corresponding effective charge on the Mn, Cr, Cu and Zn atoms in different 3d compounds. Investigation for chemical shift studies were carried out on 3d elements Mn, Cr, Cu and Zn and their compounds using Synchrotron X-ray source. K X-ray absorption edges were measured in various compounds containing Mn in Mn^{2+} , Mn^{3+} and Mn^{4+} oxidation states, Cr in Cr^{3+} and Cr^{6+} oxidation state and Cu and Zn in 2+ state in different compounds. Manu Grover from Waters India Pvt. Limited, Bangalore presented the next paper. The title of his talk was Innovations in Liquid Chromatography and Detector technology. HPLC has been adopted as standard analytical testing tool by many industries because of its versatility to analyze wide range of analytes, accuracy, sensitivity and also specificity. In pharmaceutical industry the role of HPLC has become most critical as it is used as main testing equipment to certify the quality of the product in terms of content and purity of analyte. Various models, design and make of HPLC are available in market today and transferring methods across the makes and models is critical challenge faced by industry today, Waters with their keen understanding of the analytical challenges innovated to bring in to market a unique UHPLC system with "dual flow path" technology and "gradient smart start" feature which could resolve the analytical challenges related to method transfers across HPLC systems of different design and make. The system described here is called as "Acquity Arc", it not only replicates the existing HPLC methods but also helps in modernization of analytical methods by using 2.5 μ m columns in same system.

Technical Session IV after lunch was chaired by Dr D.K.Singh, REDS, Materials Group, Bhabha Atomic Research Centre, Trombay, Mumbai. Dr R.S.Jayasree from Biophotonics and Imaging Division of Sri Chitra Thirunal Institute for Medical Science and Technology, Trivandrum was the first speaker. The title of her talk was, "Raman Spectroscopy - An Emerging Tool for Modern Biomedicine". According to her the Raman "signature" signals from the inelastic scattering of

normal bonds of cells and tissues can be very well identified from that of disease states. This enables the use of this technique for designing diagnostic devices. However, the presence of intrinsic tissue auto-fluorescence and the very low signal to noise ratio always hinder Raman responses and have to be taken care and addressed. By adopting appropriate signal enhancing approaches and by using efficient detection system, the use of this unique technique could be strengthened in the biomedical field. Raman imaging has already proven as a good candidate for cancer diagnosis with more than 90% accuracy and sensitivity in in vivo models. With the special features, Raman spectroscopy and imaging would take over the point-of-care diagnostics in the near future. The second talk in the session was delivered by Dr Manoj G.Pillai Director-Application Support, SCIEX. He talked on Liquid chromatography Mass Spectrometry workflows for Food Analysis. In his talk he highlighted the importance of Liquid chromatography Mass spectrometry as an essential tool for residue analysis in Food. The ever increasing number and type of analytes also pushes to opt for identifying new workflows both in sample preparation and based on mass spectrometry. Multiple Reaction monitoring (MRM) based quantitation is still taking the lead for quantitation of various residues in food analysis and this makes the triple quadrupole mass spectrometer as the gold standard for the routine residue analysis. This was followed by a contributed oral presentation by Dr V.C.Ady from Radiochemistry Division of Bhabha Atomic Research Centre, Mumbai on Exploring high resolution ICP-AES for determination of common metallic impurities in Uranium Matrix, This was followed by poster session in which 54 poster papers were presented. The wealth of material covered in the poster sessions was remarkable. Among many significant contributions, five presentations were selected for the best poster awards. Dr P.N.Mohandas, Former Deputy Director, CSIRNIIST, Trivandrum and Prof. Dr Mrs Beena Mathew from School of Chemical Sciences, Mahatma Gandhi University evaluated the posters. List of award winning posters is given below:

1. AN ELECTROCHEMICAL SENSOR FOR THE DETERMINATION OF NITRITE USING PRE-TREATED GRAPHITE ELECTRODE MODIFIED WITH PAMAM DENDRIMER AND PNB

C. Lakshmi Devi ^[a] and S. Sriman Narayanan ^{[a]*}

Department of Analytical Chemistry, School of Chemical Sciences, University of Madras, Guindy Campus, Chennai 600 025, Tamil Nadu, India.

2. PHOTOCATALYTIC ACTIVITY OF GRAPHITIC CARBON NITRIDES DERIVED FROM DIFFERENT PRECURSORS

Marilyn Mary Xavier¹, Dr. P. Radhakrishnan Nair¹, Dr. Suresh Mathew^{1,2}

¹Advanced Molecular Materials Research Centre,².School of Chemical Sciences, MG University, Kottayam 686560, Kerala State, India

3. FLEXI ELECTROCHEMICAL TRANSDUCERS FOR SENSING NEUROTRANSMITTERS

A. Aashish, Neethu K. S, G. Krishna Priya, U. S. Hareesh and J. D. Sudha*

Photosciences and Photonics Section, Chemical Sciences and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology, Trivandrum-695019

4. MANGROVES AS "BLUE CARBON" RESOURCE - A COMPARATIVE CASE STUDY OF MANGROVE ECOSYSTEMS OF KERALA AND WEST BENGAL WITH SPECIAL EMPHASIS ON THE MONSOON SEASON IN 2017.

Suchismita Saha¹, Anu Gopinath², Arnab Bandyopadhyay³, Greeshma K.S.⁴, Jennees Mathew⁵

1. Department of Aquatic Environment Management, K.U.F.O.S,Kochi
2. Department of Chemical Oceanography, K.U.F.O.S,Kochi.
3. Department of Fisheries Engineering and Technology, K.U.F.O.S, Kochi.
4. Soil Water Analysis Lab, K.U.F.O.S,Kochi
5. Marine Chemistry of the Department of Chemical Oceanography,CUSAT,Kochi

Kerala University of Fisheries and Ocean Studies, P.O.Panangad, Madavana Junction, Kochi-682506. Kerala.

5. ENRICHMENT FACTOR AND BIO-CONCENTRATION FACTOR OF HEAVY METALS IN COMMONLY GROWN PLANTS IN INDUSTRIAL AREA OF VISAKHAPATNAM

Tanushree Panigrahi^a , Anima Sunil Dadhich^a , M. Sudarshan^b

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Technical Session V ,commenced at 09.30 hours on 10th February 2018. This session was chaired by Dr A. Ajayaghosh, Director, CSIR-NIIST, Thiruvananthapuram. The first paper in this session was entitled," High-performance XPS with multi-technique integration. It was presented by Karthick Balasubramanian, Molecular Spectroscopy & Surface Analysis, Thermo Fisher Scientific India Pvt. Ltd., Bengaluru. Over the past decade improved instrument reliability and automation has led to the broader use of X-ray Photoelectron Spectroscopy (XPS); changing from a specialist technique only performed by dedicated practitioners to a routine analysis tool that is widespread throughout academia and industry. In his presentation he discussed the new Nexsa system, developed by Thermo Fisher and the many benefits it provides to the user. His presentation also discussed the different capabilities of the individual techniques and covered several applications of the technique, in metallurgy, semi-conductors and polymers. The second paper in the session was presented by Dr R.Raghavan, Former Senior Manager from Hindustan Zinc Limited. He talked on Applications of Electro-analytical techniques in Mining and Metallurgical Industries. Various electro-analytical techniques such as pH meter with precision Ion meter, potentiometric titrators, thermometric titrators, voltammetric analysers, ion-chromatography are being used at various mining and metallurgical industries as well as electroplating industries which were presented by him in his talk. The third paper was presented by Dr Roopa Bose from Atomic Minerals Directorate for Exploration and Research, Bangalore. The title of her talk was," Adsorption studies of U(VI) on synthesized Nano Crystalline Ceria from Aqueous Medium". In her talk, she described a simple co - precipitation method used by her for the lab preparation of ceria nano-crystals which were then applied to study the adsorption behavior of the adsorbent towards uranium in aqueous medium. A systematic study of the optimization parameters to obtain the maximum adsorption capacity has been carried out. The mechanism of adsorption is predicted based on the isothermal and kinetic modeling. Different spectroscopic techniques used for characterization of the nanocrystals was also discussed. The

scope of this methodology for large scale applications based on the reusability and regeneration of the nano adsorbent was also discussed.

Technical Session VI was chaired by Dr P.N.Mohandas, former Deputy Director, CSIR-NIIST, Thiruvananthapuram. The first talk in the Session was presented by Prof.N. Rajesh from BITS-Pilani, Hyderabad Campus. He talked on the Role of cellulose, clays, polymeric resins and graphene in heavy metal remediation. In his talk he presented analytical characterization of biodegradable and customized adsorbent materials involving cellulose, graphene oxide and clay materials for the sequestration of the stable oxidation states (hexavalent and trivalent) of chromium from waste water. Second paper in the session was presented by Dr Annie Thomas from Heavy Water Board, Department of Atomic Energy, Mumbai. The title of her talk was, "Deuterated compounds as NMR solvents". Presently D-labeled compounds including NMR solvents are being imported. Heavy Water Board initiated developmental work at their plant in Baroda and has established a lab scale synthesis and purification facility. This facility produces Chloroform-d, DMSO- d₆, Acetone- d₆, Benzene -d₆ etc. Process development work undertaken by them for producing the above labeled compounds and non nuclear applications of heavy water was discussed by her in this talk. Dr Benny George from ASCG, Vikram Sarabhai Space Centre ,Thiruvananthapuram was the next speaker. He spoke on Applications of Spectroscopic Techniques in Space Science and Technology". In his talk he described analytical techniques, including spectroscopic methods are extensively used in space exploration and launch vehicle/satellite technology-Starting from the characterization of materials like propellant raw materials, adhesives, paints, composites, etc. to functional level evaluation of space components and to space explorations (e.g. detection of water on Moon), applications of spectroscopic techniques in space technology is endless. His lecture gave a bird's eye view of the applications of different spectroscopic methods in space science and technology. Apart from illustrating the application of various spectroscopic techniques in the characterization/quality control of materials, the role of advanced techniques like thermal desorption-mass spectrometry, Atomic Force Microscopy-Raman spectroscopy, UV-VIS-NMR Spectrometer connected with integrating sphere for the measurement of solar absorption, Raman imaging for characterization of interphases, etc. were also discussed. The last paper in the Session was presented by Dr D.K.Das from Radiometallurgy Division , Bhabha Atomic Research Centre, Mumbai. "Application of Microwave in Nuclear Fuel Processing", was the title of his presentation. The second stage of three stage nuclear power programme in India is based on plutonium bearing fuels. It has been perceived that significant quantity of scrap is likely to be generated during fabrication of this fuel. This needs to be recycled & reused judiciously since scrap material is very important both from production and inventory point of view. Dry recycle of the rejected fuel pellets by conventional techniques has limitation in achieving the required physical characteristics. R&D work has been carried out by his group to develop the microwave based process as an alternative technique for the above purpose. Results were presented by him in his paper.

After Lunch Technical Session VII was started. Dr R.Rajeev, Head Analytical and Spectroscopy Division, VSSC, Thiruvananthapuram chaired this Session. In this session five contributed papers selected for oral presentations were presented. Details of the papers are given below:

1. YSZ - PuO₂ System: Inert Matrix Fuel Candidate.

Chiranjit Nandi, K. Bhandari, S. Bhattacharya, D K Das, A. Prakash and V Bhasin

Radiometallurgy Division, Bhabha Atomic Research Centre, Mumbai- 400085

2 Marine macroalgae mediated biosynthesis of multiapplicative silver and gold nanoparticles

Princy.K.F¹, Anu Gopinath²

¹Department of Chemistry, Govt.Polytechnic College, Kalamassery, Kerala, India

²Department of Fishery Hydrography, Kerala University of Fisheries and Ocean Studies, Cochin, India

3. Electrochemical impedance spectroscopy (EIS) analysis for lithium ion battery

Bijoy Kumar Das, R. Prakash, R. Gopalan

International Advanced Research Centre for Powder Metallurgy & New Materials (ARCI)

IIT-M Research Park, 6 Kanagam Road, Taramani, Chennai-600113, India.

4. Studies on Liquid metal corrosion of Austenitic Steels in Lead-Bismuth Eutetic(LBE) using Microscopy and Electrochemical methods.

Chintamani Das

Materials Group, Bhabha Atomic Research Centre, Trombay, Mumbai-400085

5. Cyclometalated Ir (III) complex as a lysosome targeted potential sensitizer for photodynamic therapy and bioimaging.

K. V. Sudheesh and Dr. A. Ajayaghosh

Chemical Sciences and Technology Division and Academy of Scientific and Innovative Research (AcSIR), CSIR-National Institute for Interdisciplinary Science and Technology (CSIR-NIIST), Trivandrum-695019, India

Among the above, Presentation No 5 was adjudged to be the best oral presentation.

The concluding session started at 16.00 hours and was chaired by Dr A.Ajayaghosh, Director-CSIR-NIIST, Thiruvananthapuram. He spoke on the importance of scientific conferences such as IASC 2018 in creating awareness among scientists, technologists and particularly students about the innovations and emerging advances in analytical science and technology. He suggested that ISAS should continue to organize similar conferences and workshops for the benefit of students and researchers. He urged the participants and organizers to spread the awareness and knowledge gained by them in the conference to make India a powerful nation in the area of science and technology. Shri S.K.Malhotra President ISAS promised the delegates and dignitaries present during the concluding session that ISAS will continue to work for the

advancement of analytical science and technology in our country and also continue to organize similar conferences and workshops. Dr Ganapathy Ramakrishnan, Dr Daisy Joseph, Dr NK Pillai, Dr P.P Chandrachoodan, Dr Suresh Mathew, and Dr VR Nair also spoke on the occasion. There was a feed back session in which the participants voiced their opinions and comments. All those who attended the conferences agreed that the event was well organized and papers presented were of a very high standard, the sessions very lively and useful for the delegates.

Overall, IASC 2018 was a highly interdisciplinary conference where innovations and emerging advances in the area of analytical science and technology were discussed in a congenial atmosphere. The conference was well organized and enabled optimum interaction between the delegates and experts and provided lots of networking opportunities. Scientists and experts from all over the country, dealing with various aspects of chemistry ,physics, biology , technology and engineering, participated in the congress. The grand success of the conference has motivated the organizers to go ahead with organizing more such programmes to elevate analytical science and technology to greater heights in our country.