Orissa Chemical Society

First OCS Extended Lecture Series 2020

International Conference on

'Recent Advances in Chemical Science'

28th and 29th November 2020

Proceedings

Organized by

Department of Chemistry

Dhenkanal Autonomous College, Dhenkanal

Dhenkanal Autonomous College, Dhenkanal

Program

Day 1

28th Nov 2020, Saturday

Inaugural Session: 10.30 – 10.50 AM

Session Chair: President, OCS

10.30 – 10.35 AM	**Dr. Shashadhar Samal** President Orissa Chemical Society	Welcome address
10.35 – 10.40 AM	**Dr. (Mrs.) Rashmi Mishra** Principal Dhenkanal Autonomous College	Address by the Patron of the conference
10.40 – 10.45 AM	**Dr. Priyaranjan Mohapatra** Secretary-cum-Treasurer Orissa Chemical Society	Scope and importance of OCS extended lecture series
10.45 – 10.50 AM	**Dr. Debasis Mohanty** Convenor OCS Extended Lecture Series	Exposing front-line research to students in peripheral educational institutions

TECHNICAL SESSIONS

Technical Session I

Session Chair: Dr.(Mrs.) Subasini Lenka

10.50 – 11.30 AM	Keynote Address **Prof. P. K. Iyer** IIT Guwahati	Designing Functional Materials for Sensors, Optoelectronics, and Healthcare Applications
11.30 – 12.00 Noon	Plenary Lecture 1 **Prof. S. K. Sahoo** SVNIT Surat	Fluorescent Sensors based on Aggregation-Induced Emission
12.00 – 12.25 PM	Invited Talk **Dr. R. Sarma** University of Kentucky USA	Bio-inspired Membranes: Application Towards Pollutant Degradation and Value-Added Transformation

Technical Session II

Session Chair: Prof. Satyaban Jena

12.25 – 12.50 PM	Invited talk **Dr. S. K. Rout** Ludwig-Maximilians-Universität München, Germany	New Approaches for Organic Synthesis may Apply to Drug Discovery
12.50 – 01.15 PM	Invited talk **Dr. M. Sahoo** Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamilnadu	An introduction to X-ray Absorption Spectroscopy: Delineating Nitrogen Location in N-TiO_2-thin films

Panel Discussion Session

Session Chair: Prof. Gopabandhu Behera

01.15 – 01.30 PM	**Panel Discussion** Day 1 Closing Remarks by Session Chair

For further details, please contact:
Dr. Debsis Mohanty, Convenor, OCS-Extended Lecture Series, E-Mail maildebasismohanty@gmail.com Phone: +919861391190
Dr. Priyaranjan Mohapatra, Secretary-cum-Treasurer, OCS, priya_chem@vssut.ac.in, racs.dkl@gmail.com Phone +919337046418

Day 2

29th Nov 2020, Sunday

Technical Session III

Session Chair: Prof. Bijaya Kumar Mishra

10.30 – 11.00 AM	Plenary Lecture 2 **Prof. Aditya N. Panda** IIT Guwahati	Understanding a Bimolecular Chemical Reaction: Quantum and Classical Studies
11.00 – 11.25 AM	Invited talk **Dr. K. K. Nanda** Pontificia Universidad Católica de Chile	Chemical Energy Storage in Small Molecules
11.25 – 11.50 AM	Invited talk **Dr. B. P. Biswal** Ashoka University, Harayana	Emerging Porous Materials Towards Molecular Separation and Solar Fuel Production

Technical Session IV

Session Chair: Prof. Bhishma Kumar Patel

11.50 AM – 12.15 PM	Invited talk Dr. L. N. Nanda The Hebrew University of Jerusalem, Israel	Asymmetric Total Syntheses of Butanolide and Butenolide Natural Products Using Donor-Acceptor Cyclopropanes
12.15 – 12.40 PM	Invited talk Dr. A. Karmakar Centro de Química Estrutural, Instituto Superior Técnico	Development of Amide Functionalized Metal-Organic Frameworks for Heterogeneous Catalytic Applications
12.40 – 01.05 PM	Invited talk Dr. F. A. S. Chipem Manipur University	Computational Study on the Electronic Structure of Substituted Polycyclic Aromatic Hydrocarbons

Panel Discussion Session

Session Chair: Prof. Ashok Kumar Mishra

01.05 – 01.20 PM	**Panel Discussion** Day 2 Closing remarks by Session Chair
01.20 – 01.30 PM	**Closing Function** Closing remarks by President, OCS Announcement of Next OCS Event by the Secretary, OCS Vote of Thanks by Dr. D. Mohanty, Convenor, OCS Extended Lecture Series

Panel Chairs

Day 1, 28.11.20
01.15 – 01.30 PM

Prof. Gopabandhu Behera
Professor of Chemistry (Retd.)
Sambalpur University, Burla

Day 2, 29.11.20
01.05 – 01.20 PM

Prof. Ashok Kumar Mishra
Professor and Dean Academics
IIT, Madras

PANELISTS

Prof. Smruti Prava Das
Professor
Ravenshaw University
Cuttack

Prof. Sagar D. Delekar
Professor
Shivaji University
Kolhapur, Maharashtra

Prof. Ajay Kumar Behera
Professor
Sambalpur University
Burla

rof. Narayan Pradhan
Professor
IACS, Kolkata

Prof. Nigamananda Das
Professor
and Director CDC
Utkal University
Bhubaneswar

Prof. Paritosh Mohanty
Professor
IIT Roorkee

Prof. Ratan Kumar Dey
Professor
and Vice-Chancellor
(Acting)
Central University,
Jharkhand

Prof. Sarat Kumar Swain
Professor
and Dean Academics
VSSUT, Burla

The participants can ask questions in the interactive window.

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Principal, Dhenkanal (Auto) College

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Head of the Department of Chemistry

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About Orissa Chemical Society

The Orissa Chemical Society (OCS) is a non-profit scientific society registered under the Societies Registration Act, 1860. The Society, conceptualized in the School of Chemistry, Sambalpur University, was established in 1985 with late Professor Mahendra Kumar Rout as the founder president. The members of the Society are from diverse disciplines of chemical science. The society aims to enhance the quality of teaching and research in chemistry in Odisha and popularise it among the students and the state's general public. Since its inception, the OCS has consistently grown in strength by attracting members from inside and outside the state, including overseas members. The Society organizes regular regional and annual conferences. For the first time, the OCS is organizing OCS Extended Lecture Series, starting with the present international conference (webinar) on 'Recent Advances on Chemical Science', hosted by Dhenkanal Autonomous College, Dhenkanal, Odisha.

About Dhenkanal Autonomous College

Situated in the sylvan setting of forest, hills, and mango groves, Dhenkanal Autonomous College is a premier college of Odisha. Established in 1959 at the backdrop of a picturesque landscape, the college has carved a niche for itself in academic excellence in the state and the country. The Department of Chemistry is one of the oldest departments of the college. The department has made a hallmark in chemistry teaching since its inception. The department's vision is to impart knowledge to students through effective teaching and inspire them to take chemistry as a career. The department offers a three-years degree course in Bachelor of Science. The courses have been designed as per Choice Based Credit System (CBCS) prescribed by Utkal University. The institution is the feeder college for all the reputed universities of the state and all leading national institutes like central universities, the NITs, and the IITs.

About the Conference on 'Recent Advances in Chemical Science'

The human being is now facing many challenges for its existence. It is now realized that sustainable development necessitates a balance between material growth and the environment. Without a healthy ecosystem, human civilization would plunge into a massive crisis like the current COVID19 pandemic. Chemical science is known to provide solutions to various challenges faced by human Society for the last several centuries. For over a century, many breakthrough discoveries have been made by chemical scientists across the globe to ease human life. This international conference on 'Recent Advances in Chemical Science' aims to expose the audience to current science. In this series, many scientists of national/international repute from various parts of the world will deliver talk on recent developments in chemistry.

Dr. Shashadhar Samal
PRESIDENT, OCS

Message

In recent years, with the establishment of new national-level institutes and universities, Odisha is witnessing an unprecedented growth in higher education and research. These institutes of national importance have excellent infrastructure. In addition to the new institutes and universities, the existing ones are being upgraded. There is a vast pool of researchers in these temples of higher learning who are working in diverse disciplines of chemical sciences. From the quality of publications, it is seen that chemistry research in Odisha has taken a quantum jump and fast attaining international standards. Therefore, the members of the chemistry fraternity of the state must meet frequently and exchange ideas.

The OCS Extended Lecture Series is formulated with the vision of getting the chemistry fraternity updated with the advances in chemical sciences in the state and appraise our position *vis-à-vis* the global scenario. In the lecture series, speakers from diverse disciplines are invited to present their work. I am sure the participants will be amply benefited from the lecture series.

Initially intended for holding the meeting in-person, the current COVID19 pandemic requires that it be held online. The First OCS Extended Lecture Series is being organized by Dhenkanal Autonomous College, Odisha on 28th and 29th November, 2020. I offer my sincere thanks to the Principal of the College, Dr. Rasmi Mishra, for this good gesture in granting permission to hold the meeting. I congratulate Dr. Priyaranjan Mohapatra, Secretary-cum-Treasurer, OCS, Dr. Debasis Mohanty, Convener of the Meet, and all the members of the Organizing Committee for holding this historic conference in a virtual platform. I am confident that the meeting will be a grand success with the kind of dedication and hard work shown.

Best wishes,

(Shashadhar Samal)
President, OCS

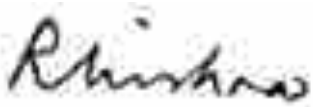
Dr. Rashmi Mishra
PRINCIPAL
Denkanal Autonomous College

Message

Department of Chemistry is one of the leading departments of Dhenkanal Autonomous College. The department has always been setting benchmarks not only in teaching but also in other academic and non-academic activities. Department of Chemistry, led by its Head of the Department, is the pioneer and front leader in organizing virtual seminars. Inspired by them, other departments of the colleges have also organized several national and international seminars. It gives me immense pleasure that the chemistry department will organize an international seminar in collaboration with the Orissa Chemical Society on the topic '*Recent Advances in Chemical Science*'. I am confident that the virtual conference will encourage the students of peripheral colleges to take chemistry as a career. In this platform, they will learn about the vast scope to build a career in chemical science, and their morale will get a boost by interacting with eminent scientists of international repute from across the globe. I am also very much happy to know that a bulletin will be published after the conference. I feel it pertinent to mention that the Department of Chemistry regularly publishes seminar bulletin 'The Catalyst' and wall magazine 'Aroma'. These are providing platforms to the budding scientist of the department to express their creative and innovative ideas.

I wish all success to the First OCS Extended Lecture Series 2020 and the International Conference on 'Recent Advances in Chemical Science'.

Thank you,



(Dr. Rashmi Mishra)
PRINCIPAL

Dr. Priyaranjan Mohapatra
Associate Professor, VSSUT, Burla
Secretary-cum-Treasurer, OCS

Scope and Importance of OCS Extended Lecture Series

The functioning of the Orissa Chemical Society is guided by its bylaw with the primary objective of augmenting teaching and research in Odisha. Since its inception, the Society has been organizing various seminars and symposia in its Regional and Annual Conferences. In these conferences, all the memorial and award lectures are held. Over the years, the OCS has grown in strength, as seen by a steady increase in the number of abstracts received for oral and poster presentations. Given the time constraints, only a limited number of invited lectures and some student presentations are accommodated. With an increase in the number of the memorial and award lectures, time allocated for student presentations is getting further curtailed. It is realized that the OCS should undertake some new initiatives that can ease the burden on the Annual Conference. The OCS Extended Lecture Series is created for this purpose.

In recent years, there is a rapid surge of chemistry research in the state in most of the technical and non-technical institutes. It is important to take stock of the developments through frequent interactions. Such meetings could serve the young researchers and students by exposing them the latest developments. The OCS, being an apex scientific body of the state, could be a common platform for scientific deliberations.

The First OCS Extended Lecture Series 2020 is organized with eleven lectures. The speakers are from diverse branches of chemical sciences. The meeting is being held in virtual platform on 28th and 29th November, 2020 on the conference title 'Recent Advances in Chemical Science'. The meeting is being hosted by Dhenkanal Autonomous College, Odisha. It is hoped that the students all over the state and country will find the webinar informative and useful. As it is the first of its kind for the OCS, our initial experience will guide us to refine our strategy for such meetings in future. In this context, the feedback of the participants will be a guiding factor. The OCS will remain committed to consistently organizing meetings with quality presentations in all its future endeavours.

Dr. Debasis Mohanty
Head, Department of Chemistry
Dhenkanal Autonomous College
CONVENOR

Exposing front-line research to students in peripheral educational institutions

I am expressing my gratitude to the President of OCS and other OCS members for introducing the innovative idea of the OCS Extended Lecture Series, and Dhenkanal Autonomous College is given the opportunity to organize the first meeting. This will be immensely beneficial to the undergraduate and postgraduate students of peripheral educational institutions. The students will be exposed to the latest advances in chemical science and get the opportunity to interact with researchers and academicians of national and international repute. They will be inspired to take chemistry as a career. Before five to six years, an undergraduate student of chemistry of the college preferred to do MBA, MCA, B.Ed., and nursing instead of post-graduation in chemistry. The trend has been changing a little bit after exposing them to the vast world of chemistry and the opportunities awaiting them by arranging regular interactive seminars with academicians of national and international repute. More and more students opt for post-graduation in chemistry and aim to build a career in chemical science. This lecture series will be a step in the right direction. Our students are now selected in the leading state universities and central universities, and other institutes of national repute for post-graduation in chemistry. This year, one of our students has been selected in Jawaharlal Nehru University while two in Central University, Hyderabad, three in other CUs, and two others in Delhi University. Six of our students have secured ranks within 100 in the recently conducted common entrance examination for state universities. Still, there is doubt in the minds of the students and their parents of these peripheral regions about a chemical science career. Hence this type of conference boosts the student's confidence to opt chemistry as a career. Especially seminars like this in the virtual platform is a boon to the students of peripheral colleges. In a physical forum, colleges like Dhenkanal College can't get so many resource persons and participants from across the globe. Hence we must be thankful to the COVID19 pandemic for opening up this new avenue of the conference on virtual mode.

We are very much thankful to Orissa Chemical Society for allowing us to conduct the first lecture series. It is a very proud moment for Dhenkanal Autonomous College to organize such a virtual conference. More than 575 participants have registered for this conference in different parts of the country and overseas. Out of the participants, 45% are undergraduate and postgraduate students, and another 12% are research scholars. Again 68 % of the participants are non-OCS members. These statistics give me a positive vibe as an organizer and provide the satisfaction that the message will reach the targeted audience. It is an opportunity for OCS to spread its aim and objective to the whole country and attract many others to join OCS and expand its horizon. An innovative concept of the panel discussion on the topic '**The Role OCS Can Play in Supporting Chemistry Teaching and Research in Academic Institutions of Odisha'** will help enhance the research culture in peripheral colleges.

TECHNICAL SESSIONS

Technical Session I
Session Chair: Dr. Subhasini Lenka

10.50 – 11.30 AM	Keynote Address **Prof. P. K. Iyer** IIT Guwahati	Designing functional materials for sensors, optoelectronics and healthcare applications
11.30 – 12.00 Noon	Plenary Lecture 1 **Prof. Suban K. Sahoo** SVNIT Surat	Fluorescent Sensors based on Aggregation-Induced Emission
12.00 – 12.25 PM	Invited Talk **Dr. Rupam Sarma** University of Kentucky USA	Bio-inspired Membranes: Application Towards Pollutant Degradation and Value-Added Transformation

Dr. Subhasini Lenka
OCS President 2013

Prof. P. K. Iyer
IIT Guwahati

Prof. Suban K. Sahoo
SVNIT Surat

Dr. Rupam Sarma
University of Kentucky USA

Keynote Address

Designing Functional Materials for Sensors, Optoelectronics and Healthcare Applications

Parameswar Krishnan Iyer*

*[1]Department of Chemistry, [2]Centre for Nanotechnology, Indian Institute of Technology Guwahati, Guwahati-781039, Assam, India. *Email: pki@iitg.ac.in*

New functional luminescent dyes based on the principle of aggregation-induced emission (AIE) have been designed and developed. They have been utilized for chemosensors, biosensors, bioimaging, optoelectronic devices, and latent fingerprinting applications. By introducing specific functional groups, aggregation caused quenching (ACQ) molecules were converted to bright AIE/AIEE dyes, which were utilized as excellent platforms in solution as well solid phase for the detection of important analytes of relevance to environment, cancer therapeutics, anti-amyloid activity as well as wash-free bioimaging applications. These organic dyes and functional materials displayed strong self-assembling nature in water, in crystalline and amorphous forms on desired surfaces, in physiological environment allowing them to be applied as sensors, healthcare probes and optoelectronic devices. This lecture will present the design principles that were utilized to develop several advanced materials and their remarkable applications by introducing functional group engineering.

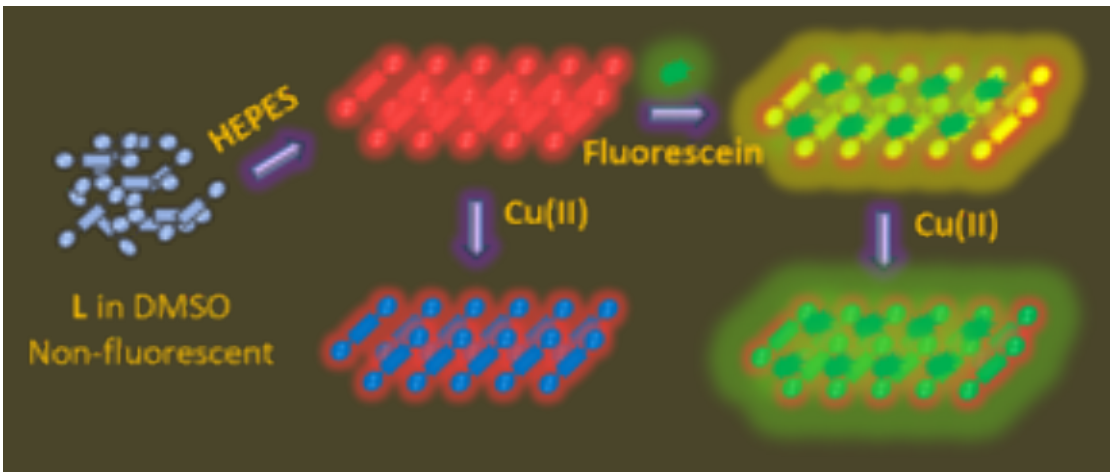
Plenary Lecture 1

Fluorescent Sensors based on Aggregation-Induced Emission

Suban K Sahoo

Department of Applied Chemistry, Sardar Vallabhbhai National Institute of Technology, Surat 395007, India. E-mail: sks@chem.svnit.ac.in; subansahoo@gmail.com.

There is bourgeoning interest in the current years for the development of aggregation-induced emission luminogen (AIEgen) for their advantageous properties of excellent photostability, good biocompatibility and high emission efficiency. The AIEgens are also extensively applied in the field of fluorescent sensing and biosensing [1-3]. In this presentation, the fabrication of AIE active Schiff base L derived using vitamin B_6 cofactor pyridoxal by reacting with 1,4-diaminobenzene in 2:1 ratio was discussed. The ligand L insoluble in aqueous medium but soluble in organic solvents like DMSO, EtOH, CH_3CN etc. Pyridoxal based probe is a AIE active and shows a weak fluorescence in DMSO, while the fluorescence was markedly enhanced with increasing poor solvent fraction and exhibits distinct behaviour in different ratio of DMSO:HEPES. This novel red-emitting AIEgen L shows a good fluorescence turn-off response towards Cu^{2+} ion with the excellent limit of detection of 2.7 μM, and the estimated LOD is much lower than that of US Environmental Protection Agency (EPA) permitted in drinking water. The developed AIE active luminogen was also applied for the various real sample application such as river water, tap water and biological samples such as saliva and urine with the good recovery %. Further, the red-emitting AIEgen L was mixed appropriately with fluorescein or green-emitting nanoclusters, and converted into a Cu^{2+} selective ratiometric fluorescent sensor.



References

1. Sahoo *et al.,* Pyridoxal derived AIEgen as a fluorescent pH sensor, *Dyes and Pigments,* 2020, accepted.
2. Sahoo *et al.*, Decorating vitamin B_6 cofactor over beta-cyclodextrin stabilized silver nanoparticles through inclusion complexation for fluorescent turn-on detection of hydrazine,*ACS Applied Bio Materials*, 2020, accepted.

Invited Talk 1

Bio-inspired Membranes: Application Towards Pollutant Degradation and Value-Added Transformation

Rupam Sarma

Department of Pharmaceutical Sciences,University of Kentucky, Lexington, KY40506
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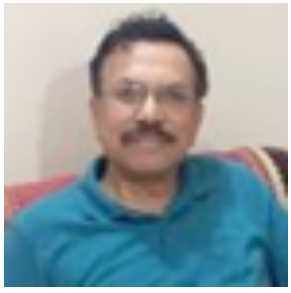
Bio-inspired membrane with immobilized enzymes on it provides versatile platforms for applications ranging from environmental remediation to generation of value added chemicals from waste. Despite associated environmental concerns, the existing techniques for remediating pollutants in water consist of both physical and chemical means mostly using heavy metals. To offer bioremediation as an alternative option, we herein demonstrate a layer-by-layer approach to immobilize enzyme into functionalized membranes. This mode of membrane functionalization provides a synergistic platform for pollutant degradation where leaching of heavy metals into the environment is unacceptable. The enzyme-functionalized membrane was characterized by a wide variety of spectroscopic and microscopic techniques including ATR FT-IR, SEM imaging and XPS analysis and more. The stability of the enzyme in both solution phase and on membrane phase was studied. Enzyme showed a loss of some 65% of initial activity in the solution phase after weeks of use, whereas the membrane-bound enzyme lost only a negligible percentage of activity in the same time span. Activity of these biomimetic membranes towards dechlorination of 2,4,6-trichlorophenol (TCP) is demonstrated under pressure driven continuous flow mode. Up to 80% of the initial TCP was degraded at optimum flow rate. The membrane was exposed to rigorous cycles of TCP exposure to study its long term activity and reusability. The primary results reveal that our laccase-functionalized membrane lost only 14% of its initial activity in a period of 25 days. Finally, the reusability of the membrane as a support material was also demonstrated by detaching and re-immobilizing the enzyme on the membrane-polymer domain for multiple consecutive cycles.

We have further extended the layer-by-layer approach to fabricate multienzyme functionalized membrane reactor for bioconversion of lignin model compound involving enzymatic reactions. Three different enzymes (glucose oxidase, peroxidase and laccase) were immobilized into functionalized PVDF membranes. This novel membrane reactor couples the in-situ generation of hydrogen peroxide to oxidative conversion of a lignin model compound, guaiacylglycerol-B-guaiacylether (GGE). Preliminary investigation of the efficacy of these functional membranes towards GGE degradation is demonstrated under convective flow mode. Over 90% of the initial feed could be degraded with the multienzyme immobilized membranes. GGE conversion product analysis revealed formation of oligomeric oxidation products with peroxidase, which might be potential hazard to membrane bioreactors. These oxidation products could be further degraded by laccase enzymes in the multienzymatic membranes explaining the potential of multienzyme membrane reactors.

I acknowledge the support from University of Kentucky and NSF-EPSCoR program for carrying out this research.

Technical Session II
Session Chair: Prof. Satyaban Jena

12.25 – 12.50 PM	Invited talk **Dr. S. K. Rout** Ludwig-Maximilians-Universität München, Germany	New Approaches for Organic Synthesis may Apply to Drug Discovery
12.50 – 01.15 PM	Invited talk **Dr. Madhusmita Sahoo** Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamilnadu	An introduction to X-ray Absorption Spectroscopy: Delineating Nitrogen Location in N-TiO_2-thin films



Prof. Satyaban Jena
OCS President 2016

Dr. Saroj K. Rout
Ludwig-Maximilians-Universität München
Germany

Dr. Madhusmita Sahoo
Indira Gandhi Centre for Atomic Research,
Kalpakkam, Tamilnadu

Invited Talk 2

New approaches for organic synthesis may apply to drug discovery

Saroj K. Rout

Ludwig-Maximilians-Universität München, Germany
Email: saroch@cup.uni-muenchen.de

(**A**) **Strain ring in drugs, how to introduce them in molecules?** Bicyclo[1.1.1]pentane (BCP) replacement as a bioisostere in drug has an influence on their permeability, aqueous solubility and invitro metabolic stability[1,2]. Thus, the chemical installation of the BCP unit into a chemical entity remains a significant challenge from a synthetic point of view. Here, we have presented a new approach for the installation of the BCP unit on the xanthate moiety by means of a radical exchange process[3,4]. (**B**) **Unactivated esters in Mannich reaction**: An organocatalyzed direct Mannich reaction of unactivated α-styrylacetates was realized for the first time by using a quinidine C6'-urea catalyst, the direct Mannich reaction of a styrylacetates and N-tosylimines gave the desired β-amino ester in high yields, distreoselectivities and *ee* values[5]. (**C**) **C-H functionalization as an emerging tool**: My research work was focussed on the development of methodologies for the construction of carbon-carbon and carbon heteroatom bonds via oxidative functionalizations of un-activated sp^2 and sp^3 C-H bonds using transition metal catalysts with the assistance of directing groups. In addition to this, extensive mechanistic investigations have been carried out to deduce the mechanistic scenario of these transformations[6-12].

Reference

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5. J. Guang, S. Rout, M. Bihani. J. A. Larson, H. D. Arman and J. C. –G. Zhao, *Org. Lett.,* **2016**, *18*, 2648.
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12. A. Gogoi, A. Modi, S. Guin, S. K**.** Rout, D. Das and B. K. Patel, *Chem. Commun.,* **2014**, 50, 10445.

Technical Session III
Session Chair: Prof. Bijaya K. Mishra

10.30 – 11.00 AM	Plenary Lecture 2 **Prof. Aditya N. Panda** IIT Guwahati	Understanding a Bimolecular Chemical Reaction: Quantum and Classical Studies
11.00 – 11.25 AM	Invited talk **Dr. K. K. Nanda** Pontificia Universidad Católica de Chile	Chemical Energy Storage in Small Molecules
11.25 – 11.50 AM	Invited talk **Dr. B. P. Biswal** Ashoka University, Harayana	Emerging Porous Materials Towards Molecular Separation and Solar Fuel Production

Prof. Bijaya Kumar Mishra
OCS President 2015

Prof. Aditya N. Panda
IIT, Guwahati

Dr. K. K. Nanda
Pontificia Universidad Católica de Chile

Dr. Bisnu Prasad Biswal
Ashoka University, Harayana

Plenary Lecture 2

Understanding a bimolecular chemical reaction: Quantum and classical studies

Aditya N. Panda

Department of Chemistry, Indian Institute of Technology Guwahati
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A simple reaction of the type A + BC $\longrightarrow$ AB + C can proceed through either a direct (instant), an indirect (time-delayed) or a combination of both mechanisms. In this talk, I will present the results of exact quantum dynamical studies of three representative reactions, Br + HD $\longrightarrow$ BrH + D and H^- + HD $\longrightarrow$ HD (H_2) + H^-(D^-). Based on these results, the involvement of any of these mechanisms and their effects on the observables will be discussed. Quantum effects and the applicability of classical mechanics to study these mechanisms will also be discussed.

Invited Talk 4

Chemical Energy Storage in Small Molecules

Kamala Kanta Nanda* [a,b]

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The rigorous consumption of fossil fuels for energy and transportation, resulting in excessive emission of pollutants, which exacerbate global environmental problems.[1] There is an urgent need to develop clean energy technologies that generate power and fuels from renewable sources like solar and wind energy. However, the intermittent and diurnal nature of wind and solar energy sources makes it indispensable to devise an efficient method of energy storage to mitigate the gap between global energy supply and demand. Batteries and supercapacitors may be used to store the energy produced, but they have lower volumetric and gravimetric energy densities and can only scale up to MW size.[2] The comparison between various energy storage technologies in the sense of storage capacity and discharge power duration reveals that chemical energy storage in the form of chemical bonds in energy-rich compounds has enormous potential.[2]
Electrolysis converts electrical energy into chemical energy *via* redox reactions and storing electrons in the form of stable chemical bonds. The chemical energy can be used as a fuel (by combustion) or converted back to electricity (in a fuel cell) when needed. Therefore, electrolytic reactions such as water and CO_2 electrolysis can potentially enable renewable energy storage in chemical bonds of the product molecules. In water electrolysis, hydrogen and oxygen are produced. The hydrogen is used as fuel for automobiles and used for generating electricity in a fuel cell device. On the other hand, CO_2 can be electrolyzed to synthetic gas (CO and H_2), hydrocarbons, and fuels such as formic acid, ethanol, etc. in a multi-electron reduction process. These electrochemical processes can be driven by solar energy, and the process is termed artificial photosynthesis. Artificial photosynthesis systems use semiconductors as a photocatalyst to perform photo(electro)catalytic water splitting and CO_2 reduction, which generates clean, energy-dense fuels such as hydrogen, methane, methanol, etc.[3] This presentation will discuss design and development, such as renewable energy storage systems. A brief overview of the role of the surface structure of the catalyst in determining the mechanism of product formation and product selectivity will be presented. Further, to enhance the energy efficiency of such systems, the strategy to replace thermodynamically unfavorable water oxidation half-reaction with alternative oxidation reactions will be discussed. [4]

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Invited Talk 5

Emerging Porous Materials Towards Molecular Separation and Solar Fuel Production

Bishnu P. Biswal

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Porous crystalline frameworks (PCFs) such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) are gaining increasing attention as new-age materials due to their diverse practical applications in gas storage, separation, catalysis, sensing, etc.[1] Despite such advancement, chemical stability and synthetic difficulty are the two major challenges, which hinder their applicability. Moreover, storage, separations, and catalytic conversion of gases to value-added chemicals are becoming very important for many industrial applications. Although, PCFs have characteristics to be a good candidate for gas separation and photocatalysis,however, they are scarcely explored. Therefore, easy and scalable methods to synthesize these porous materials and their application as membrane materials for gas separation and photocatalytic fuel production remains a key challenge. In our research, we emphasize on simple design and easy synthesis of chemically stable MOFs and COFs;[2]their polymer composite membranes to enhance molecular separation performance[3] and engineering them for solar-driven renewable fuel production[4].

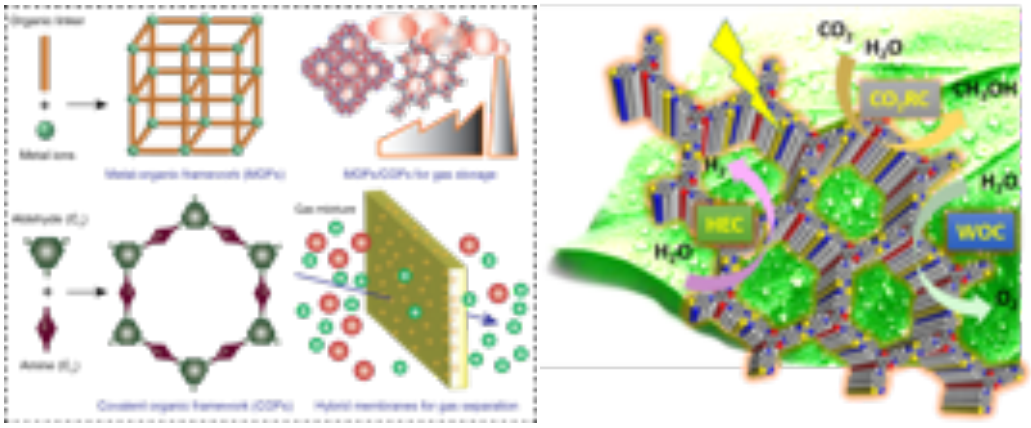

Figure 1 Advanced porous materials for molecular separation.

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Technical Session IV
Session Chair: Prof. Bhishma Patel

11.50 AM – 12.15 PM	Invited talk Dr. L. N. Nanda The Hebrew University of Jerusalem, Israel	Asymmetric Total Syntheses of Butanolide and Butenolide Natural Products Using Donor-Acceptor Cyclopropanes
12.15 – 12.40 PM	Invited talk Dr. A. Karmakar Centro de Química Estrutural, Instituto Superior Técnico	Development of Amide functionalized Metal organic frameworks for heterogeneous catalytic applications
12.40 – 01.05 PM	Invited talk Dr. F. A. S. Chipem Manipur University	Computational Study on the Electronic Structure of Substituted Polycyclic Aromatic Hydrocarbons

Prof. Bhishma Kumar Patel

Dr. L. N. Nanda
The Hebrew University of Jerusalem, Israel

Dr. A. Karmakar
Centro de Química Estrutural, Instituto Superior Técnico

Dr. F. A. S. Chipem
Manipur University

Invited Talk 6

Asymmetric Total Syntheses of Butanolide and Butenolide Natural Products Using Donor-Acceptor Cyclopropanes

Laxmi Narayan Nanda, Santosh J. Gharpure*

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Donor–Acceptor substituted cyclopropanes (D-A cyclopropanes) are fast emerging as versatile building blocks in organic synthesis.[1] Due to the push-pull effect of these donor and acceptor substituent, they show remarkably diverse reactivity with very high selectivity for cleavage of one of the cyclopropane bond sandwiched between donor and acceptor groups.[2] Not surprisingly, this interesting reactivity of D-A cyclopropanes has been exploited in the synthesis of various bioactive natural products. Lactone bearing natural products display lot of structural diversity and also varied biological activity. The five membered γ-lactone unit containing butanolides and butenolides are quite prevalent among the bioactive natural products. This presentation will address a general and divergent asymmetric total synthesis of these butanolide and butenolide natural products using oxygen substituted D-A cyclopropanes as chiral synthons.[2]

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Invited Talk 7

Development of Amide functionalized Metal organic frameworks for heterogeneous catalytic applications

Anirban Karmakar

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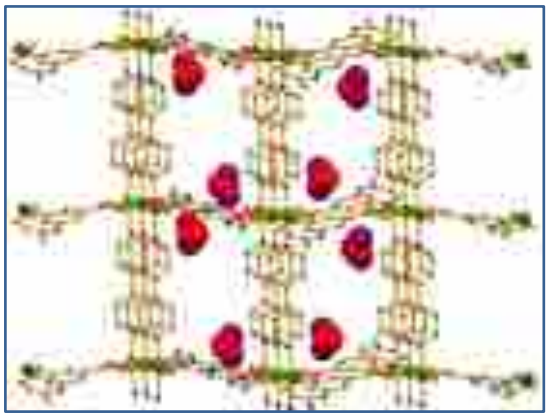
Metal–organic frameworks (MOFs) are crystalline coordination networks consisting of metal ions or clusters and multidentate organic ligands[1]. This area of research is currently undergoing a rapid growth due to their potential applications as functional materials in heterogeneous catalysts, magnetism, nonlinear optics, gas storage and separation, etc[2]. Moreover, MOFs constructed from amide based linkers have attracted considerable attention due to their interesting topologies as well as catalytic properties[3]. Thus, we have synthesized various amide functionalized multifunctional carboxylate ligands and employed them for the construction of MOFs having different dimensionality. Solvothermal/ hydrothermal reactions of different transition metals with these ligands in presence or absence of an auxiliary ligand gives rise to a series of 1D, 2D and 3DMOFs. We have characterized them by X-ray single crystal diffraction, elemental microanalysis, IR spectroscopy, thermogravimetric analysis and powder X-ray diffraction analysis. These MOFs act as effective heterogeneous catalysts for various organic transformations, for example Knoevenagel condensation, Henry, transesterification, Oxidation and Cascade type reactions under mild conditions and can be recycled without losing activity.



Representative example of a 2D MOF obtained by the reaction amidoisophthalic acid linker and a Zn(II) salt.

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Acknowledgements

This work has been supported by the Foundation for Science and Technology (FCT), Portugal (projectUID/QUI/00100/2019). AK also thanks to Instituto Superior Técnico and FCT for Scientific Employment contract (Contrato No: IST-ID/107/2018) under Decree-Law no. 57/2016, of August 29.

Invited Talk 8

Computational Study on the Electronic Structure of Substituted Polycyclic Aromatic Hydrocarbons

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π-π Stacking interaction, a strong noncovalent interaction, is the main factor for aggregation of graphene layers and, specifically, polycyclic aromatic hydrocarbons (PAHs) which are the most abundant carbonaceous molecules found in the interstellar system and can be considered as building blocks of graphene. To understand the network of carbon atoms and electronic structure in PAHs due to π-interaction, coronene molecule which is neither large to require high computational costs nor too small was theoretically examined at the level of density functional theory. Heteroatom nitrogen and boron substituted coronenes were also studied. The calculations show that the band gap of substituted monomer coronenes reduce to 0.82-1.13 eV from 3.24 eV of unsubstituted monomer coronene. Further, the extend of decrease in band gap depends on the position of substitution. The monomeric planes are stacked together by π-interactions to form different types of dimers. The dimerization due to π-π stacking stabilize the coronene dimers by upto 200 times. The band gaps of the dimers are further reduced attributing to π-π stacking interactions and the reduction is more in nitrogen substituted coronene dimers. The presentation explores polymorphism exhibited by coronene as a result of various types of dimers formed.

Panel Discussion Sessions

Panel Chair

Prof. Ashok Kumar Mishra

IIT, Madras

PANELISTS

Prof. Smruti Prava Das
Professor
Ravenshaw University, Cuttack

Prof. Sagar D. Delekar
Professor
Shivaji University
Kolhapur, Maharashtra

Prof. Bhisma K. Patel
Professor
IIT, Guwahati

Prof. Narayan Pradhan
Professor
IACS, Kolkata

Prof. Nigamananda Das
Professor
and Director CDC
Utkal University Bhubaneswar

Prof. Paritosh Mohanty
Professor
IIT Roorkee

Prof. Sarat Kumar Swain
Professor
and Dean Academics
VSSUT, Burla

Panel Discussion
Day 1

"The Role OCS Can Play in Supporting Chemistry Teaching and Research in Academic Institutions of Odisha"

Panel Chair

Prof. Ashok Kumar Mishra

Panel Members who participated in the discussion are: Prof. Smruti Prabha Das, Prof Sagar Delekar, Prof S. K. Swain and Prof Paritosh Mohanty.

Prof. Shashadhar Samal - President OCS and Prof. A. C. Dash, contributed to the discussions significantly.

Summary of Discussion:

Point 1: The discussion was in the context of the inadequacies of the current chemistry teaching/research infrastructure/manpower in a large number of academic institutions of Odisha.

Point 2: For the institutions, especially undergraduate and some postgraduate colleges, where meaningful research is almost impossible to carryout, it was suggested that OCS can primarily focus on providing educational support in terms of conducting online syllabi-relevant topic-based lecture series, which can be recorded and distributed to students/teachers. One of the assets of OCS is its highly experienced, knowledgeable and competent senior teachers. Their support will be invaluable in this regard.

Point 3: It was observed that though the undergraduate chemistry honours level curricula is uniform in Odisha, Curricula for postgraduate level teaching is different in different institutions. OCS can coordinate to make it uniform.

Point 4: Given the limited research related resource available, it was suggested that a group of institutions in close proximity can form a cluster to share their resources. Members of OCS in these institutions can form local working groups to coordinate within themselves and with other such working groups.

Point 5: Due to paucity of funds, OCS has not been able to support mobility of researchers for accessing good research facilities within Odisha and outside. The possibility of creating an endowment can be explored towards providing mobility support for students/teachers of institutions with inadequate research infrastructure.

Panel Discussion
Day 2

"The Role OCS Can Play in Supporting Chemistry Teaching and Research in Academic Institutions of Odisha"

Panel Chair

Prof. Ashok Kumar Mishra

Panelists participated are Prof Bhishma K. Patel, Prof. Narayan Pradhan, Prof. Smrutiprabha Das, Prof. Nigamananda Das, Prof. S. K. Swain and Prof. Paritosh Mohanty Mohanty.

Prof Shashadhar Samal, President, OCS also contributed significantly.

Summary :

The panel continued the discussions on some of the points discussed the previous day and added some suggestions to strengthen some of the points (as given in the trail mail below):

Point 2: The video records of online syllabi-relevant topic-based lecture series can be placed in OCS website for easy access of the students and teachers. Teaching videos of senior teachers of OCS can be extremely useful resources. These videos can also be archived for posterity.

It was pointed out that the 'project' component in the BSc syllabus is not being effectively handled in colleges due to possible lack of awareness of how to go about it. OCS can help in preparing guidelines for various stages of project report preparation starting with identification of a topic, and creating formats for project writing.

It was highlighted that there is a strong need for recording the UG chemistry practicals. Utkal University and Ravenshaw University have already conducted training programs on UG practicals for college teachers. The chemistry departments of these universities have come forward for creating such videos using Government funding resources. These can also be uploaded to OCS website.

Point 5: It was felt that some funding sources are required for OCS to be effective in supporting teaching/research activities in Odisha. The possibility of partnering with established institutions through MoU and accessing Government funding sources can be explored.

In addition, the following new ideas were proposed:

Point 6: A large number alumni of UG/PG institutions of Odisha have now established themselves as leading researchers in India and Abroad. Many of them are also members of OCS and have a desire to help the chemistry students/teachers of colleges in which they studied. OCS can proactively connect such alumni members with the respective colleges through the existing OCS network. Chemistry HoDs can be sensitized on the positive effects of such Alumni-student interactions, may be through online workshops (?).

Point 7: Established research institutions in Odisha and outside usually have easy access to research literature resources. Connecting Odia researchers needing access to such resources with OCS members of such institutions can be a big help.

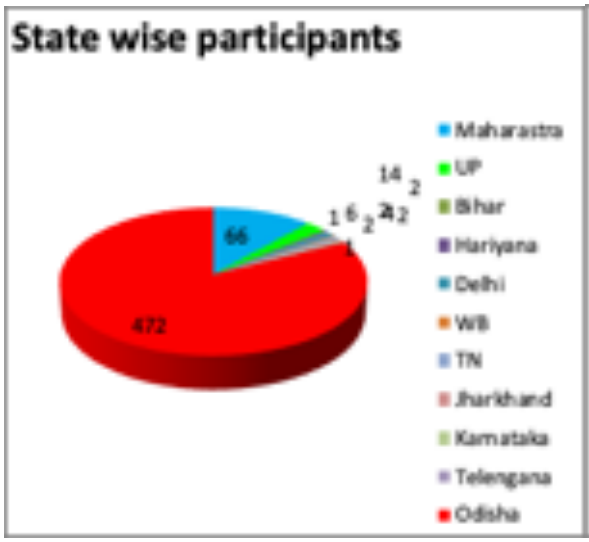
Point 8: The quality of the current design, content and layout of the OCS website was highly appreciated. It was suggested that the website can be made a rich repository of material spanning all aspects of chemistry teaching and research. It can make the website a 'go to' site for all chemists all over.

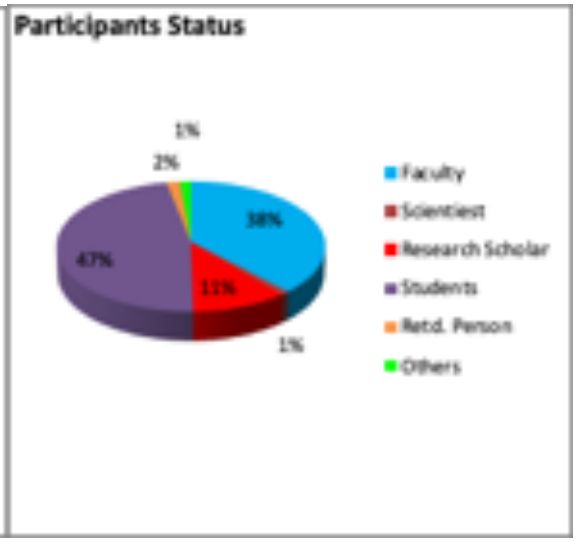
Social Media & Technology Used

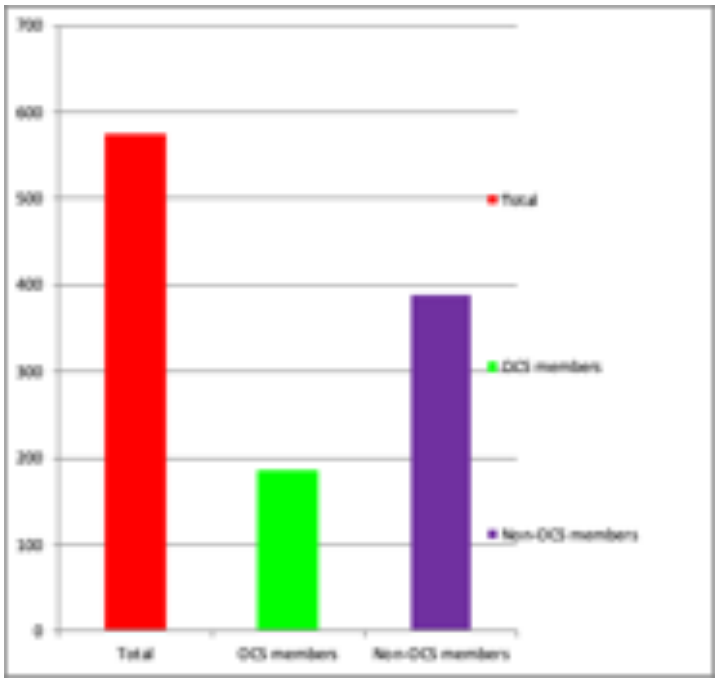
Host Platform	Zoom
Live streaming	YouTube & Facebook
Information	Facebook page, WhatsApp group and Email
Registration, Attendance and feedback	Google form
Certificate	Google slide & Certify'em
YouTube links (click the links for replay of the Live Stream)	Day 1 https://youtu.be/EDlKgg1Cvp0 Day 2 https://youtu.be/M9eudkmyBtI
Facebook Page	Department of Chemistry, Dhenkanal (Auto) College
WhatsApp Group	OCS Lecture Series

Statistics

	Participants	Speakers
Total	575	11
Indian	572	6
Overseas	3	5
Odisha	472	Nil
Other States	100	6+5







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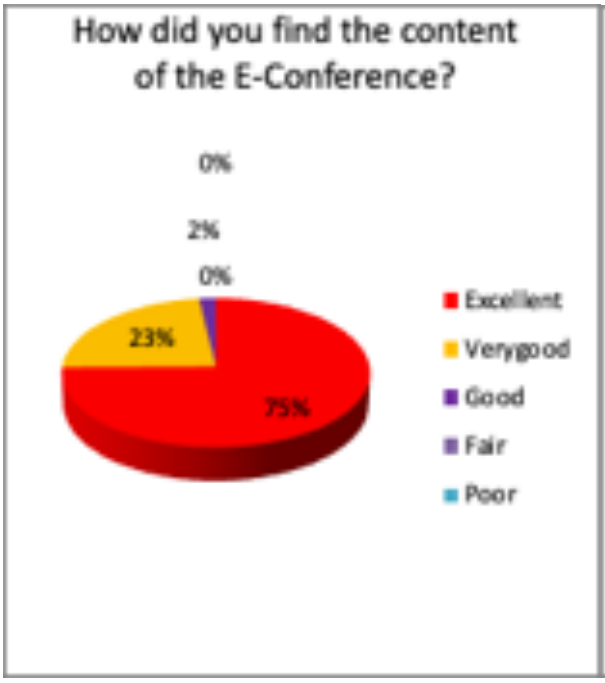

Media Coverage


The SAMAJ, Angul edition

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