# Proceedings

## SECOND OCS EXTENDED LECTURE SERIES 2021

**and the sixth series of the national conference**

## 'Recent Advancement in Materials Science'

**(RAIMS-2020)**

**22nd - 24th January 2021**

**organized by**

## Orissa Chemical Society

**Regd. No. 18990/28-87/XXVII-22/87 of 1987 – 1988**

**Website: https://www.ocs.org.in**

**in collaboration with**

## Department of Chemistry

## Veer Surendra Sai University of Technology

## Burla, INDIA


# Veer Surendra Sai University of Technology
# Burla, INDIA

# SECOND OCS EXTENDED LECTURE SERIES 2021
## and the sixth series of the national conference
## 'Recent Advancement in Materials Science'
## (RAIMS-2020)

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# Important Information on the Webinar

## Registration Link:

**https://docs.google.com/forms/d/1pwtC3XMkzNqteNH4B_4Tw6cN-F7e360GJUa7EsU2ivw/edit**

## Scan QR Code or Click on the following Link to Join in the Webinar WhatsApp Group:

1. The registered participants will be provided with the web link (ZOOM platform) 24 hours before the webinar each day.
2. The ZOOM link will be active from 9 AM on 22nd January 2021 and from 9.30 AM on 23rd and 24th January 2021.
3. During the webinar, the registered participants requiring a certificate will be provided with the attendance form each day and a feedback form at the end of the conference.
4. Those who attend the webinar on both days will be issued a participation certificate that will be emailed to their respective emails(the email I.D. provided by the participant in the feedback form).
5. The participants will also be requested to provide feedback, for which an online form will be made available.
6. The webinar will be streamed live on YouTube, the link of which will be provided.
7. For further details/clarifications, please contact:

## OCS - RAIMS2020 Secretariate

Dr. Priyaranjan Mohapatra, Secretary-cum-Treasurer, OCS,
priya_chem@vssut.ac.in, ocsindia.secretary@gmail.com Phone +919337046418
Dr. Bigyan Ranjan Jali, Assistant Professor, Department of Chemistry, VSSUT Burla
E-mail: raims.vssut@gmail.com Phone: 08249023455

## About Orissa Chemical Society

The Orissa Chemical Society was constituted in 1985 under the leadership of Prof. Mahendra Kumar Rout, renowned Professor of Chemistry of international repute and an educational administrator. The aims and objectives of the Society are to (i) promote and improve the standard of chemistry teaching in Odisha, (ii) promote chemistry research, and allied sciences in Odisha, (iii) organize conference and symposia to improve teaching and research in chemistry, (iv) popularize chemistry discipline and to create public awareness regarding environmental impacts of the use of various chemicals/chemical products in our daily life, (v) honor the eminent teachers and the chemists of Odisha, and (vi) bring out a journal in chemistry, to spread creativity among young scholars. More than 1500 chemists are the Life and Patron Members of Society. O.C.S. organizes Annual, Regional Conferences, OCS Extended Lecture Series, and OCS-Industry Interface Meet each year and offers many awards to the young chemists for their achievement in chemistry.

## About VSSUT, Burla

Formerly known as University College of Engineering (established in 1956), now transformed to Veer Surendra Sai University of Technology (VSSUT), the University was established by the Government of Odisha in 2009. It is a UGC-recognized Unitary Technical University. The University, known for its quality teaching, research potential, and eminent faculty, is a premier Government Institute of Odisha. This Institute has sculpted its standard amongst the country's best technical institutions, having more than 20,000 graduates and 3,000 postgraduate engineers, serving in reputed organizations worldwide as its alumni. An internationally acclaimed technical university, it imparts advanced technical education and provides a vibrant research enterprise to create quality engineers and researchers as world-class leaders. The Institute promotes technological innovations to serve the global community to improve the quality of life.

## About Department of Chemistry, VSSUT, Burla

The Department of Chemistry, VSSUT, Burla, established in 1956, is one of the state's oldest Chemistry Departments. The department is engaged in providing a high-quality academic environment. It has a galaxy of highly qualified faculty members having expertise in teaching and research in frontier areas with significant research output in the forms of patents, books, book chapters, and research papers. The department also gets funding for the research projects from various Government organizations and many consultancies from nearby industries. The department offers 2-year M.Sc. (Industrial & Organic Chemistry), 5-Year Integrated M.Sc., M.Phil., and Ph.D. programs.

## About the Webinar

The webinar, integrating the Second OCS extended Lecture Series and the National Conference Series RAIMS-2020, is organized by the Department of Chemistry, VSSUT Burla. RAIMS-2020 is the sixth such event of the RAIMS series being organized by the department since 2013, presenting renowned scientists and academicians in the last five meets. The present conference aims to exhibit the research and technical excellence of scientists and technocrats, representatives from academia and researchers on diverse aspects of recent advances in materials research, including but not limited to, synthesis of nanomaterials and their applications, materials for biological, energy, optical and electromagnetic applications, functional materials, engineering materials, composite materials, magnetic materials, and related topics. This conference aims to bring together globally renowned research professionals. It will include keynote and invited lectures delivered by eminent speakers. We hope that this conference will prove to be a great learning opportunity and an enriching experience for all the participants.

# Program

## Day 1: 22nd January 2021, Friday

### Inaugural Session: 09.30 – 10.00 AM

### Session Chair: President, O.C.S.

**Dr. Shashadhar Samal**

PRESIDENT, OCS

09.30 – 09.35 AM: Welcome Address

**Prof. Atal Chaudhuri**

Vice-Chancellor, VSSUT

09.35 – 09.40 AM: Welcome Address

**Prof. Uma Ranjan Jena**

Dean CDCE, VSSUT

09.40 – 09.45 AM: Welcome Address

**Dr. Priyaranjan Mohapatra**

Head, Dept. of Chemistry, VSSUT

Secretary-cum-Treasurer, OCS

09.45 – 09.50 AM: Vision of OCS EXTENDED LECTURE SERIES

**Dr. Bigyan Ranjan Jali**

Organizing Secretary

OCS EXTENDED LECTURE SERIES and RAIMS-2020

09.50 – 09.55 AM: About RAIMS Series of Meetings in VISSUT

**Dr. A. K. Barick**

Convenor

OCS EXTENDED LECTURE SERIES and RAIMS-2020

09.55 – 10.00 AM: Briefing on the Webinar Protocols

# Day 1
# 22nd January 2021, Friday

# TECHNICAL SESSIONS

## Technical Session I: 10.00 – 11.45 AM
## Session Chair: Prof. Gopabandhu Behera

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

Prof. Jyotirmayee Dash
IACS, Kolkata

Dr. Rabindra Kumar Behera
N.I.T., Rourkela

| | | |
|---|---|---|
| 10.00 – 11.00 AM | Santi Swarup Bhatnagar Award Lecture<br>**Prof. Jyotirmayee Dash**<br>Indian Association for the Cultivation of Science, Kolkata | Small molecules, D.N.A., and Self-assembly |
| 11.00 – 11.45 AM | Invited talk<br>**Dr. Rabindra Kumar Behera**<br>National Institute of Technology, Rourkela | Facilitating Iron Acquisition from Intact Ferritin Protein Nanocage |

## Technical Session II: 11.45 – 01.15 PM
## Session Chair: Prof. Raj Kishore Patel

Prof. Raj Kishore Patel
Professor of Chemistry, N.I.T., Rourkela

Prof. Paritosh Mohanty
Professor of Chemistry, I.I.T., Roorkee

Prof. S. K. Swain
Professor and Dean Academics
VSSUT, Burla

| | | |
|---|---|---|
| 11.45 – 12.30 PM | Invited talk<br>**Prof. Paritosh Mohanty**<br>Professor of Chemistry<br>I.I.T., Roorkee | Nanoporous high surface area polymeric materials for $CO_2$ capture and utilization |
| 12.30 – 01.15 PM | Invited talk<br>**Prof. S. K. Swain**<br>Professor of Chemistry<br>and Dean Academics, VISSUT, Burla | Sustainable hybrid materials |

## End of Day 1 Technical Sessions

## Announcement: Day 2 Meeting Starts at 10 AM

# Day 2: 23rd January 2021, Saturday

## Technical Session III: 10.00 – 11.30 AM

**Session Chair:** Dr. Kadambini Sarangi

Dr. Kadambini Sarangi
Principal Scientist, CSIR-IMMT Bhubaneswar

Dr. Bamaprasad Bag
Material Chemistry Department, CSIR-IMMT Bhubaneswar

Dr. Prasana Kumar Sahoo
Material Science Centre
I.I.T., Kharagpur

| | | |
|---|---|---|
| 10.00 – 10.45 AM | Invited talk<br>**Dr. Bamaprasad Bag**<br>Material Chemistry Department, CSIR-IMMT Bhubaneswar | Molecular probes in detection technology: photophysical responses of a rhodamine derivative with hypochlorous acid, effective signal translation on to electronic read-out |
| 10.45 – 11.30 AM | Invited talk<br>**Dr. Prasana Kumar Sahoo**<br>Material Science Centre<br>I.I.T., Kharagpur | Low-Dimensional Semiconductors for Optoelectronic and Sensor Applications |

## Technical Session IV: 11.30 – 01.00 PM
## Session Chair: Prof. A. K. Patnaik

Prof. Ajaya K. Patnaik
Professor of Chemistry (Retired), Ravenshaw University, Cuttack

Dr. Bikash Kumar Jena
Principal Scientist, Materials Chemistry Department, CSIR-IMMT, Bhubaneswar

Dr. Debabrata Pradhan
Associate Professor at Materials Science Centre, I.I.T. Kharagpur

| | | |
|---|---|---|
| 11.30 – 12.15 PM | Invited talk<br>**Dr. Bikash Kumar Jena**<br>Principal Scientist, Materials Chemistry Department, CSIR-IMMT, Bhubaneswar | Nanostructured Materials for Energy Conversion and Storage Applications |
| 12.15 – 01.00 PM | Invited talk<br>**Dr. Debabrata Pradhan**<br>Associate Professor at Materials Science Centre, I.I.T. Kharagpur | Heterostructures for Hydrogen Generations |

## End of Day 2 Technical Sessions

## Announcement: Day 3 Meeting Starts at 10 AM

# Day 3: 24th January 2021, Sunday

## Technical Session V: 10.00 – 11.30 AM
## Session Chair: Prof. Pramila Mishra

Prof. Pramila Mishra
Professor of Chemistry, Sambalpur University

Dr. Rati Ranjan Nayak
Senior Scientist in the Department of Organic Synthesis and Process Chemistry, CSIR-IICT

Dr. K. C. Barick
Nanotherapeutics and Biosensors Section, Chemistry Division, BARC, Mumbai

| | | |
|---|---|---|
| 10.00 – 10.45 AM | Invited talk<br>**Dr. Rati Ranjan Nayak**<br>Senior Scientist in the Department of Organic Synthesis and Process Chemistry, CSIR-IICT | Self-Assembled Nano-Architectures of Bio-based Soft Materials and Their Applications |
| 10.45 – 11.30 AM | Invited talk<br>**Dr. K. C. Barick**<br>Nanotherapeutics and Biosensors Section, Chemistry Division, BARC, Trombay | Development of Nanostructured Materials for Cancer Theranostics |

## Technical Session VI: 11.30 – 01.00 PM
## Session Chair: Prof. Pramod Kumar Satpathy

**Prof. Pramod Kumar Satpathy**
Professor of Chemistry, North Odisha University

Prof. Sukalyan Dash
Professor of Chemistry
VISSUT, Burla

Dr. Garudadhwaj Hota
Department of Chemistry, N.I.T. Rourkela

| | | |
|---|---|---|
| 11.30 – 12.15 PM | Invited talk<br>**Prof. Sukalyan Dash**<br>Professor of Chemistry<br>VISSUT, Burla | Research activity using eggshell particles – a low-cost material with high potential applications |
| 12.15 – 01.00 PM | Invited talk<br>**Dr. Garudadhwaj Hota**<br>Department of Chemistry, N.I.T. Rourkela | Electrospun Polymer Nanofiber Materials: Surface Functionalization and Environmental Applications |

# Closing Function: 01.00 – 01.15 PM

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|---|---|
| 01.00 – 01.15 PM | Closing remarks by President, O.C.S.<br>Announcement of Next O.C.S. Event by the Secretary-cum-Treasurer, O.C.S.<br>Vote of Thanks by Convener, SECOND OCS EXTENDED LECTURE SERIES |

# SECOND OCS EXTENDED LECTURE SERIES 2021

## and the sixth series of the national conference

## 'Recent Advancement in Materials Science'

## (RAIMS-2020)

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BURLA-768018, SAMBALPUR, ODISHA, INDIA
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**Prof. Atal Chaudhuri**
VICE CHANCELLOR

# MESSAGE

It is my pleasure to extend warm welcome to all the participants for 3re days National Seminar on "2nd Extended Lecture Series Orissa Chemical Society (OCS) and Recent Advance of Materials Science (RAIMS)" held during 22nd-24th January 2021 organized by Department of Chemistry, Veer Surendra Sai University of Technology, Burla in association with Orissa Chemical Society, Odisha.

During the last few decades Science and Technology has taken the pivotal role in transforming the overall life spectrum of Society by the application of innovative ideas. Academic workshop provide platform to all stakeholders for exchanging ideas and considered absolutely necessary for all concerned, to upgrade their skills constantly in order to adopt with the emerging challenges.

I am thankful to the organizer for taking efforts in bringing up such a platform to bring scientific fraternity for deliberation, to meet the need of society.

(Atal Chaudhuri)

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**Prof. Umaranjan Jena**

Dean, CDCE

VSSUT, Burla, Odisha

# MESSAGE

I am extremely happy to know that the Department of Chemistry, VSSUT, Burla in association with Orissa Chemical Society, Odisha.is organizing 3re days National Seminar on "2nd Extended Lecture Series Orissa Chemical Society (OCS) and Recent Advance of Materials Science (RAIMS)" held during 22nd-24th January 2021.

This 3re day's National seminar will focus on various aspects of science and technology for the development of the nation. The efficient way of designing new materials requires innovative research ideas and their applications. This seminar invites the researchers, academicians and engineers all over the country to share their expertise.

I extend my greetings to all concerned and express my best wishes for the grand success of the programme.

(Umaranjan Jena)

Dr. Shashadhar Samal
PRESIDENT, O.C.S.

# *Message*

The OCS extended Lecture Series is formulated with the vision of getting the chemistry fraternity updated with the advances in chemical sciences. In recent years, with the establishment of new national-level institutes and universities, Odisha is witnessing an unprecedented growth in higher education and research. In these institutes, there is a vast pool of researchers. From the quality of publications, it is seen that chemistry research in Odisha has attained international standards. In such a scenario, it will be worthwhile if the researchers meet frequently and exchange ideas.

Dhenkanal Autonomous College, Odisha, organized the First OCS Extended Lecture Series on 28$^{th}$ and 29$^{th}$ November 2020. The present meeting is the second in series organized by VSSUT, Burla, from 22$^{nd}$ to 24$^{th}$ January 2021. The Department of Chemistry, VSSUT organizes a conference series entitled 'Recent Advancement of Materials Science (RAIMS).' This year RAIMS-2020 is combined with the Second OCS Extended Lecture Series.

I offer my sincere thanks to Prof. Atal Chaudhuri, honorable Vice Chancellor, VSSUT, and Prof. Uma Ranjan Jena, Dean, VSSUT, to host the international conference. I congratulate Dr. Priyaranjan Mohapatra, Secretary-cum-Treasurer, OCS and Head of Chemistry Department, VSSUT, Dr. Bigyan Ranjan Jali, Organizing Secretary, Dr. Arun Kumar Barick, Convener of the Second OCS Extended Lecture Series and RAIMS-2020, and all the members of the Organizing Committee for holding this conference on a virtual platform. At the meeting, twelve speakers from diverse disciplines are invited to present advances in materials science. I am sure the participants will be amply benefited from the lecture series.

In post COVID era, the world will not be the same again, and so will be our approach to chemical science. It is desired that new materials are made through environment-friendly routes. The role of chemists will be pivotal in maintaining a healthy balance between environmental management and the global economy.

I wish the organizers great success,

(Shashadhar Samal)
President, O.C.S.

Dr. Priyaranjan Mohapatra
Secretary-cum-Treasurer, O.C.S.
Head, Department of Chemistry
Chairman, Organizing Committee,
RAIMS

***The vision of 'OCS EXTENDED LECTURE SERIES' and 'RAIMS Series of Lectures'***

The Orissa Chemical Society since its inception has been organizing various seminars and symposia in its Regional and Annual Conferences. 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. The First OCS Extended Lecture Series 2020 was held in virtual platform on 28$^{th}$ and 29$^{th}$ November, 2020.

It was organized by Dhenkanal Autonomous College, Odisha. The present meeting is the second in series organized by VSSUT, Burla, from 22$^{nd}$ to 24$^{th}$ January 2021. Every year, the Department of Chemistry, VSSUT organizes a conference series entitled 'Recent Advancement of Materials Science (RAIMS).' This year RAIMS-2020 is combined with the Second OCS Extended Lecture Series.

Our initial experience guided us to refine our strategy for the present second OCS Extended Lecture Series. Several distinguished speakers are invited to present their research. The winner of Santi Swarup Bhatnagar Award Prof. Jyotirmayee Dash is invited to deliver the award lecture on the topic 'Small molecules, D.N.A., and Self-assembly'. Similarly, all other lectures are of high quality and informative. I am sure, the Lecture Series will be very beneficial to the young students. The OCS will remain committed to consistently organizing meetings with quality presentations in all its future endeavours.

Dr. Priyaranjan Mohapatra
Secretary-cum-Treasurer, OCS

Dr. Bigyan Ranjan Jali
Organizing Secretary
OCS EXTENDED LECTURE
SERIES and RAIMS-2020

***About RAIMS Series of Meetings in VISSUT***

I would like to personally welcome each of you to the sixth edition of our National conference series on Recent Advance of Materials Science, and 2nd extended lecture series of Orissa Chemical Society, "OCS-RAIMS-2020". It is an exciting time for scientists, academicians and researchers, as we continue to grow and adapt systematic constructive on design of novel biomaterials and their application in day-to-day life.

I would like to thank each of you for attending OCS-RAIMS-2020 and bringing your expertise to this awesome gathering. You, as researcher, have the vision, the knowledge, the resources and the experience to help us pave our way into the future technical activities. Throughout this conference, I request you to stay engaged, keep us proactive and help us bringing out more such events in future. My personal admiration and gratitude goes out to all of you.

I sincerely thank the Hon'ble Vice-Chancellor, Prof Atal Chaudhuri, President OCS, Prof. Sasidhar Samal, HOD Chemistry, Dr. Priyaranjan Mohapatra, Dean Academics, Prof. S. K. Swain, Dean CDCE, Prof. U. R. Jena, Convener, Dr. A. K. Barick and other distinguished professor department of Chemistry and staff members of department of Chemistry, VSSUT Burla and OCS, Odisha India for hosting OCS-RAIMS-2020 in an impressive manner.
I appeal to the research community to extend their continued support and cooperation to the future activities of RAIMS and OCS-RAIMS.

BRJali

(Bigyan Ranjan Jali)

Invited Lecture 1

Santi Swarup Bhatnagar Award Lecture

# Small molecules, D.N.A., and Self-assembly

Jyotirmayee Dash

*School of Chemical Sciences, Indian Association for the Cultivation of Science, Kolkata-700032*
*E-mail: ocjd@iacs.res.in*

In the first half of this talk, I would discuss our work on the development of new methods for the synthesis of small molecules like carbazoles and pyridoindoles using ring-closing metathesis (RCM).[1,2] We have also developed new methods to synthesize different classes of compounds like indoles and carbazoles.[3] Small heterocyclic compounds are known to bind DNA and alter its function. These small molecules are considered as potential anticancer agents. Next, I will discuss our efforts on developing different classes of ligands to target DNA quadruplex, a four stranded DNA secondary structure.[3] DNA secondary structures play key regulatory roles in biological system. Targeting the DNA secondary structure by small molecules could provide new therapeutic strategies. We have shown that DNA can be used as a template to synthesize its own ligands by Target Directed Synthesis.[4] Natural nucleosides present in DNA can self-assemble to mimic DNA secondary structures. The last part of my talk would focus on our work on self-assembly of nucleosides to form hydrogels and ion channels.[5]

## References

1. (a) T. Mandal, G. Chakraborti, S. Karmakar, J. Dash, Org. Lett. 2018, 20, 4759. (b) K. Dhara, T. Mandal. J. Das, J. Dash, Angew. Chem. Int. Edn., 2015, 54, 15831.
2. (a) T. Mandal, G. Chakraborti, S. Maiti, J. Dash, Org. Let. 2019, 21, 8044. (b) G. Chakraborti, S. Paladhi, T. Mandal, J. Dash, J. of Org. Chem. 2018, 83, 7347.
3. P. Saha, D. Panda, J. Dash, Chem. Commun. 2019, 55, 731-750.
4. (a) P. Saha, D. Panda, D. Müller, A. Maity, H. Schwalbe, J. Dash, Chem. Sci. 2020, 11, 2058. (b) D. Panda, P. Saha, T. Das, J. Dash, Nat. Commun. 2017, 8, 16103.
5. T. Bhattacharyya, P. Saha, J. Dash, A.C.S. Omega, 2018, 3, 2230.

**Prof. Jyotirmayee Dash**, Indian Association for the Cultivation of Science, Kolkata, bagged the Santi Swarup Bhatnagar Prize 2020 in the area of Chemical Sciences. She is a Professor, School of Sciences, IACS and the recipient of Prof. R. C. Tripathy Award 2014, is the first Odia female scientist to win this prize. Dr. Jyotirmayee Dash has obtained her Ph.D. degree in Organic Chemistry from Indian Institute of Technology, Kanpur, India under the supervision of Professor F. A. Khan. She has been awarded Alexander von Humboldt postdoctoral fellowship to continue her research in the group of Professor H.-U. Reissig at Freie University, Berlin, Germany. She has joined the research group of Professor Janine Cossy at ESPCI, Paris, France as a postdoctoral research fellow and subsequently has been awarded Marie Curie postdoctoral fellowship in the research group of Professor Shankar Balasubramanian, University of Cambridge, UK. She has returned to join Indian Institute of Science Education and Research, Kolkata as an Assistant Professor in 2009. She moved to at the Indian Association for the Cultivation of Science-Kolkata in 2012, where she is currently working as a Professor. Her research interests include new organic transformations, structure and function of nucleic acid targets in therapeutics and nanotechnology. She has published more than hundred publications, two book chapters and 6 patent applications.

**Awards and Honours**

Editorial Advisory Board Member, *A.C.S. Omega*, 2021
International Advisory Board, *Asian J.O.C.*, 2021
Editorial Advisory Board Member, *ChemComm*, 2020
Shanti Swarup Bhatnagar Prize, 2020
Fellow of the Royal Society of Chemistry, FRSC, 2020
Selected for CRSI Bronze Medal, 2020
D.B.T./ Wellcome Trust Indian Alliance Senior Fellowship, 2020
Second Charusita Chakravarty Memorial Lecture, February 2019, CRSI India
Swarna Jayanti Fellowship for the year 2015-2016

Invited Lecture 2

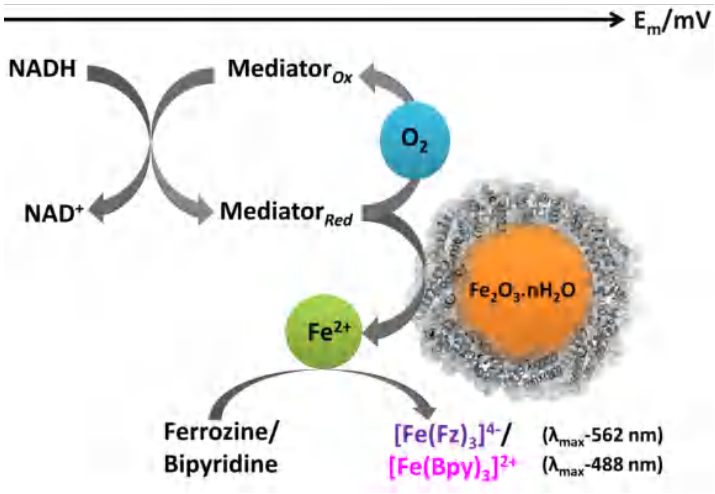
# Facilitating Iron Acquisition from Intact Ferritin Protein Nanocage

Rabindra K. Behera

*Department of Chemistry, National Institute of Technology, Rourkela 769008, Odisha, India*
*E-mail: beherarabi@nitrkl.ac.in.*

Iron is vital to almost all organisms owing to its participation in various physiological functions such as electron transfer (ATP synthesis, photosynthesis and $N_2$ fixation), DNA synthesis and oxygen transport [1]. While the cellular requirement of iron ranges from $10^{-6}$ M to $10^{-3}$ M, the Fe(III) solubility under physiological conditions is only ~ $10^{-18}$ M [2,3]. Ferritins decrease this gap inside the living cells via protein-coated hydrated ferric oxy (hydroxide) mineral ($Fe_2O_3.xH_2O$) [2,3,4]. Ferritin core can store ~ 4500 iron atoms, achieving iron concentration equivalent to ~ 0.2 M. However, free Fe(II) ions, regarded as toxic, creates oxidative stress in the cells via Fenton reaction [3]. Therefore, iron behaves as a double-edged sword i.e. beneficial as well as harmful, depending upon its form (free or bound) and its cellular level.

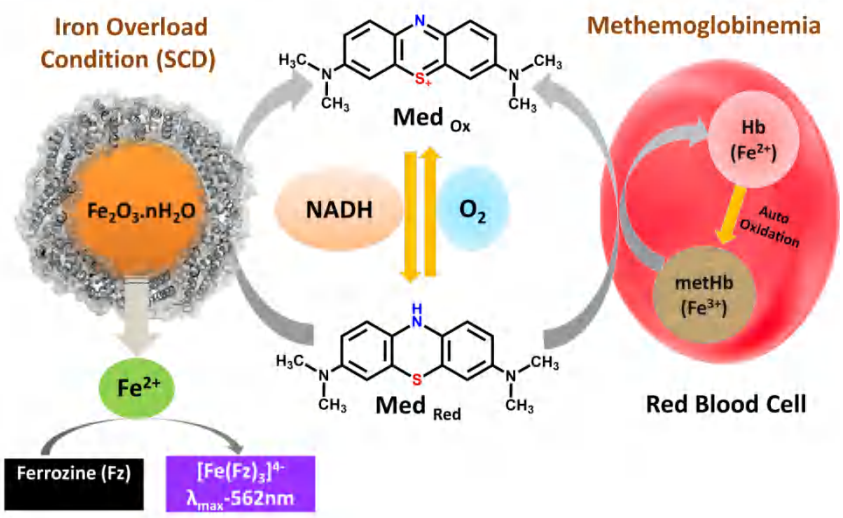
Ferritins are hollow spherical proteins, encoded by almost all organisms. These supramolecular protein architectures are self-assembled from 24 folded polypeptide subunits [1-7]. The labile, highly toxic, free Fe(II) ions are sequestered rapidly (in few msec to sec) by these ferritins to synthesize ferrihydrite ($Fe_2O_3.xH_2O$) mineral in their central nanocavity via protein mediated complex oxidative/hydrolytic (biomineralization) reaction. About 2 nm thick, ferritin protein cage encapsulates the iron mineral thereby preventing its unwanted leakage by cytoplasmic reductants [1]. However, upon cellular requirement, iron is released in a controlled way for various cellular and metabolic activities.




**Scheme 1** Facilitating reductive iron mobilization from ferritin by using electron mediators.

*In vivo,* what kind of cytoplasmic signals and regulation exists for iron mobilizations from ferritin mineral core is not well known. *In vitro,* the low solubility of ferric mineral at neutral pH and its encapsulation by stable ferritin nanocage limits iron release, although some pathogen can acquire it by unknown mechanism [4]. Moreover, physiological reducing agents were inefficient in releasing the ferritin iron, when used alone [5-7]. Therefore, a series of electron relay molecules (mediators) were employed along with reducing agent to facilitate the iron mobilization process [**Scheme 1**]. Flavins

(phenazine based biological electron transfer mediators) and phenothiazines/phenoxazines (synthetic electron mediator used during treatment of methemoglobinemia; **Scheme 2**) were known to works well




in association with its redox partner, N.A.D. (P)H.

**Scheme 2** Learning from methemoglobinemia treatment to facilitate iron mobilization from ferritin (by exploiting the role of E.T. mediator).

Similar to Marcus ET theory, our observations suggest that the mediators with $E_{1/2}$ values well separated from those of the reducing agents and of the ferritin mineral can be exploited not only to facilitate iron removal during biological iron overload conditions but also explains the microbial iron acquisition process.

## References


1. Theil, Tosha and Behera., *Accounts of Chemical Research.*; 2016, 49, 784-91.
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Invited Lecture 3

# Nanoporous high surface area polymeric materials for $CO_2$ capture and utilization

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Burning of "fossil fuels" produces huge amounts of gaseous products while providing the required energy that have large scale impact on the environment. Moreover, the detrimental environmental effect associated with the extraction, purification/production, and use of fossil fuels goes beyond tailpipe emissions.[1a,b] In fact, the geologically sequestered "fossil fuels" added to the biosphere contaminants is highly inimical to human life. Not only that, other downstream processes to produce various chemicals and finished products created pollutants that were never existing before on earth.[1b]

Inspired by the nature and history of the development of human civilization, the current trend in solving the energy and environmental issues lie mostly on finding suitable materials and technological use of these for a sustainable growth. For example, to address the global warming effect, which is mainly due to the excess $CO_2$ content in the atmosphere that reaches as high as 414 ppm in the recent time, tremendous efforts are being made to find suitable adsorbents such as liquid organic amines and various high surface area solids that can separate $CO_2$ from the flue gas stream, and also materials which can efficiently convert $CO_2$ to value added products. [1c-e] However, due to one or other drawbacks, none of these processes is commercially sustainable at present. Still continued efforts in this direction are made in research and development of superior adsorbents which can capture and convert large quantity of $CO_2$. High thermodynamic stability ($-\Delta H_f = -394$ kJ/mol) of $CO_2$ is a bottleneck for its conversion to targeted products, hence, its activation by appropriate materials is required. Although, metal-based materials are popular choices, however, cost, abundance and environmental concerns owing to metal ion leaching has encouraged to explore their metal-free counterparts.[1e]

Different approaches were adopted to increase the $CO_2$ capture and conversion capacity that include the increase in the specific surface area, pore volume and use of various surface functionalities. Moreover, inclusion of electron rich heteroatoms such as N, P, O, etc. in the high surface area nanoporous polymeric materials, which could interact strongly with Lewis acidic gas such as $CO_2$ leading the research due to the encouraging outcome both from the theoretical investigation and experimental studies.[2a] In this direction, various metal-free heteroatoms enriched high surface area nanoporous materials have been synthesised in our group by conventional as well as non-conventional approaches. Materials such as H.N.M.s, P.H.M.s, CHNM, CPMOs, IBNF, HCPANIs, NENPs, MNENP, PT@SBA-16, PAH have shown $CO_2$ capture capacity of 4.29, 1.83, 5.18, 2.19, 5.27, 3.67, 7.68, 2.2, 1.28, 4.79 mmol $g^{-1}$ at 1 bar pressure and 0 °C.[2b-g,3] Among all the specimens, NENP which has high N content of 52 wt% has shown the maximum $CO_2$ uptake of 7.68 mmol $g^{-1}$ at 1 bar pressure and 0 °C, The higher $CO_2$ sorption capacity of the synthesised specimens has indicated a strong affinity towards $CO_2$ due to the presence of heteroatom such as N which act as Lewis base and interact with $CO_2$ via Lewis acid-Lewis base interaction.[3a] However, at higher pressure of 30 bar, the PAH has shown a maximum $CO_2$ capture capacity of 37.9 mmol $g^{-1}$ at 0 °C.

Among several series of nanoporous metal free high surface area materials, the heteroatoms enriched materials such as MNENP, NENP, PT@SBA-16, NENP, H.N.M. and CHNM have been explored for the utilization of $CO_2$ owing to an enhanced Lewis acid-base interaction with the $CO_2$ molecules.[2c-d,3]The use of $CO_2$ to react with epoxides for the synthesis of cyclic carbonates, which has got a lot of

applications in pharmaceuticals and chemical industries, have got tremendous interest to the scientific community. The cycloaddition of $CO_2$ with different epoxide substrates such as epichlorohydrin, epibromohydrin, 1,2-epoxy hexane, propylene oxide, styrene oxide and glycidyl phenyl ether with different functionality were investigated. The reaction was carried out at mild to moderate experimental condition of 100 °C and 4 bar of $CO_2$ pressure with a varying reaction time of 12 to 36 h, depending upon the catalysts used. A high conversion of *ca.* 100% and high selectivity was observed in most of the experiments. In most pf the cases, the catalyst showed good recyclability with retention of almost 90 % of its activity after five cycles. The superior activity of the synthesised specimens can be attributed to multiple factors such as high $SA_{BET}$, hierarchical pore structure, large and uniform distribution of task-specific functionality. The presence of –OH and –NH functionalities play their respective roles by interacting with the epoxide and $CO_2$ molecules via H-bonding and Lewis acid-Lewis base interactions, respectively. The plausible mechanism is also proposed for the formation of cyclic carbonates via cycloaddition of epoxides and $CO_2$. Also, the MNENP has been explored for electrochemical conversion of $CO_2$ to value added products and it was found to be active for the conversion of $CO_2$ to $CH_3OH$, CO and $CH_4$, electrochemically.

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**Dr. Paritosh Mohanty** is presently serving as a Professor in the Department of Chemistry, IIT, Roorkee**.** He completed M.Sc. from Ravenshaw College (Autonomous) then affiliated to Utkal University, Odisha, in 1997, and completed Ph.D. from IIT Kharagpur in 2004 working on mesoporous alumina and composites. He spent two years (2004-2006) in the Department of Chemistry, KAIST, South Korea. The research area was metal nanowires and nanotubes. From 2006 to 2010, he worked as postdoctoral research associate, Research Scientist-III and Senior Research Scientist in the Department of Chemistry at Lehigh University, U.S.A. On return to India, he joined IIT Roorkee in 2011 as Assistant professor, got promoted to Associate Professor in 2015, and in August 2020 he became a full Professor. His areas of research are Nanoporous materials: synthesis, characterization and applications for energy and environmental applications, $CO_2$ capture and conversion to products of industrial importance such as methane, methanol and cyclic carbonates, *etc*. Metal-free catalysis, adsorption of gases and metal ions. Cleaning of petroleum products etc. He has published around 75 papers. Notable papers are published in Nature communications, J. Am. Chem. Soc., Angew. Chem. Int. J., J. Mater. Chem. A, PNAS USA, Nanoletters, Chem. Commun., Chem. Engg. Journal, Langmuir, Environmental Sci. Nano, J. Phys. Chem. B, etc. Total citation around 1800 with h-index of 22 and i10-index of 49. Already 5 scholars have been awarded Ph.D., 10 M.Tech. and 7 M.Sc. students are graduated under his supervision. Currently 10 Ph.D. scholars and two M.S. students are working under his supervision.

Invited Lecture 4

# Nano-Structure Sustainable Hybrid Material: Past, Present and Future

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Material has created its own importance since ancient age where human beings learn to decorate and design different products for their applications. When individual materials need its novelty for targeting particular applications, it needs to combine with multiple components according to their compatibility. When two or more components are combined to make a novel material where individual components lost their properties then it is known as hybrid material. When one of the components has the resin in nanoscale then the combined material is known as nanostructured hybrid material. Due to nano dimension, material achieve new structure, morphology, orientation and properties by either intercalation or exfoliation dispersion of the material. The thermal, mechanical, gas barrier, biodegradability and chemical resistance properties are enhanced substantially due to incorporation of the nano structured material. The sustainability of the nano structured material is achieved when the hybrid material is quite eligible for various applications like sensing, super conductivity, water treatment, dye removal, smart packaging including biomedical applications. It is quite expected that smart hybrid material will be a potential candidate to meet the future challenge and solve problems of the Society.

**Prof. Sarat Kumar Swain** is currently working as a Professor of Chemistry and Dean (Academic Affairs) at Veer Surendra Sai University of Technology, Burla, Sambalpur since 2011 Before joining to present position, he was serving as an Associate Professor of Chemistry at the North Orissa University, Baripada,. He was working as Post-Doctoral Fellow in Department of Polymer Engineering, University of Akron, Akron, OH, U.S.A. after receiving his Doctoral degree from Utkal University, Bhubaneswar, India. He was also working as a visiting researcher at Indian Association for Cultivation for Science, Kolkata and Jawaharlal Nehru Centre for Advanced and Scientific Research, Bangalore with awarding INSA Fellowship and JNCASR Fellowship respectively. He has more than 20 years of experience in teaching and research in the area of Organic Chemistry, Materials Chemistry, Nanotechnology and Polymer Chemistry at UG, PG and PhD levels. His area of research interests includes, hybrid nanomaterials, reinforced polymer nanocomposites, advance materials like graphene, nanoclay, CNT, CNF for improving of gas barrier, fire retardant, thermal, mechanical and chemical resistance properties of the materials. He has designed various kinds of nanostructured materials for wastewater treatment, packaging usage, anti-corrosion performance, superconductor properties, sensor behaviors and biomedical applications. He has published more than 100 research papers in different SCI. international journals. So far he has authored 03 books, 30 book chapters, and with inventions of two patents (One USA and One Indian) to his credits. There are fifteen scholars are successfully awarded PhD degree along with 13 MPhil, 05 MTech and 25 MSc degrees with active supervisions of Prof. Swain He has also delivered several plenary and invited talks in different International conferences in India and abroad. Prof. Swain has received different awards such as BOYSCAST Fellowship, DAE-Young Scientist research award, Prof. R K Nanda award and "Samanta Chandra Sekhar Award and gold medal" for various academic achievements.

Invited Lecture 5

# Molecular probes in detection technology: photophysical responses of a rhodamine derivative with hypochlorous acid, effective signal translation on to electronic read-out

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**Abstract**: A rhodamine derivative has been developed as molecular probe for detection of hypochlorous acid with adequate selectivity and sensitivity. The detection ability of the organic material was demonstrated in a triple helical microfluidic system. The manifested photophysical signalling of the probe was further translated onto electronic circuitry output display for development of a hand-held device contributing to detection technology.

**Description:** Organic materials with capabilities of tunable photo-functional properties have been emerging as crucial contributors to molecular electronics, photonics and detection technologies. Covalently architected molecular systems, with their design driven by their specified yet changeable inter-componential interactions, have already been explored in detection of various analytes of physiological and environmental importance, particularly, those analytes which imparts detrimental impacts with their toxicity. Hypochlorous acid (HOCl) and its conjugate base ($OCl^-$) as important reactive oxygen species (ROS) are such (bio-)analytes whose detection have attracted considerable attention. HOCl is produced endogenously from hydrogen-peroxide and chloride ions through myeloperoxidase-catalyzed reactions; however, a deviation in regulation of its concentration threshold stimulates health hazards in form of various life-threatening diseases. Therefore, an on-site, real time, selective detection and quantifiable analysis of HOCl is highly desirable for monitoring and impact assessment purposes. Many analytical methods have been developed and employed for detection of HOCl, which despite of having numerous advantages, however are jeopardised with disadvantages of operational protocols and usage of sophisticated instruments. On another methodological progression, chemosensory probes with colorimetric and fluorometric signalling provide an alternative and viable solution, with their advantages of synthetic and operational protocol as well as have already proven to be a non-evasive, non-destructive and 'easy-to-handle' method. Design and development of such probes are driven by various parameters such as methodologies exploiting plausible probe- analyte interactions, perturbation of involved photophysical processes and manifestation of the output signal are the determining parameters in design and development of such signalling probes. Advantageous are those, which express the recognition event with perturbed photophysical signal at both fluorogenic and chromogenic dual channel output. Rhodamine derivatives[1] are one of such class of potential dye materials, and many rhodamine based luminescent signalling probes[1-4] have been developed exploiting its excellent spectroscopic properties which rely on a straight forward protocol of their structure-function correlation, and its ability to modulate signal in aqueous media. In an effort with the mentioned rational basis of design and development of molecular probes, a rhodamine derivative **1** was synthesized, thoroughly characterized with various spectroscopic techniques, and its photophysical spectral behaviour in both solution and solid state were investigated for selective and sensitive detection of HOCl when present in traces.

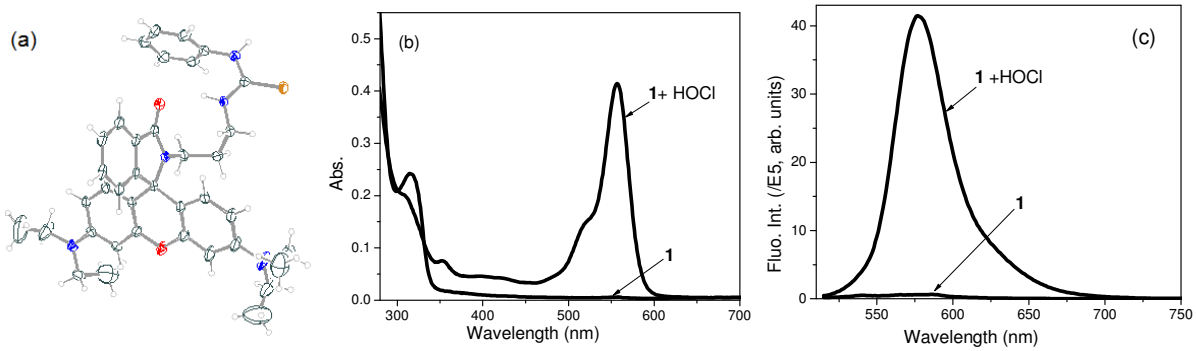


**Figure 1** (a) Structure of **1** (X-ray diffracted single crystal); Absorption (b) and Fluorescence (c) spectra of **1** alone and in presence of HOCl showing respective photophysical signal responses.

The solution of **1** in EtOH as such is colourless and non-fluorescent, however, on interaction with HOCl, it simultaneously exhibits colour transition and fluorescence enhancement, rationalized through structure function correlation.

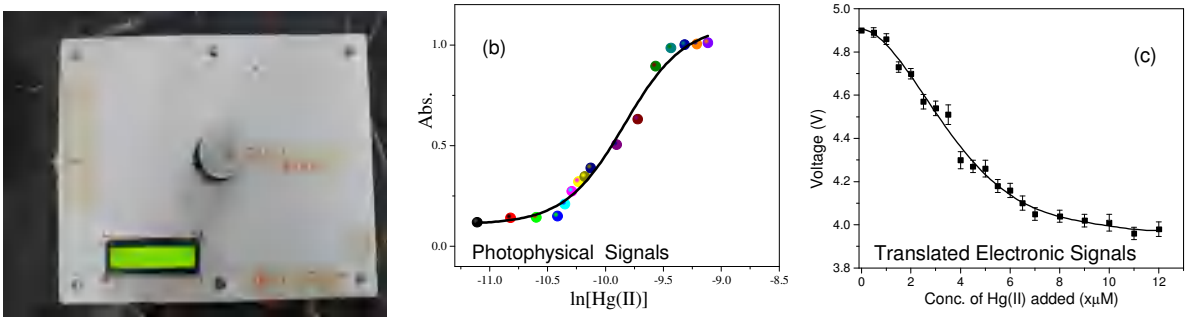


**Figure 2** (a) The fabricated device, (b) photophysical reading of the chemosensor performance and (c) corresponding electronic read-out with the developed device.

Prima-facie, an appropriate sensing platform for digitization of the optical signals/ colour mapping with requisite electronic circuitry was designed and its workability was investigated. The electronic read-out for the photophysical signals of **1** was demonstrated to exhibit stability to the signals when employed for detection of HOCl. The detailed investigation on photophysical signaling, associated operational intricacies and device development will be discussed further.

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**Dr. Bamaprasad Bag**, a BOYSCAST Fellow, Raman Research Fellow, Visiting researcher, Univ. of Strasbourg, France, joined CSIR-Institute of Minerals and Materials Technology Bhubaneswar (earlier, Regional Research Laboratory) in 2006 as Scientist and has been undertaking research independently on development of luminescent organic materials. Presently, he is Principal Scientist, Materials Chemistry Department Coordinator, AcSIR, CSIR-Institute of Minerals and Materials Technology Bhubaneswar 751 013, India. An alumnus to Ravenshaw College Cuttack, where he studied +2 (Science) and B. Sc. (chemistry honours); he had moved to School of Chemistry, University of Hyderabad (India) for M. Sc. (chemistry) and M. Phil. (chemistry) degree. He joined Prof. P. K. Bharadwaj's group at Indian Institute of Technology Kanpur (India) for his doctoral thesis where he had learned and studied molecular/supramolecular architectures, chemistry of cryptands in particular. He further had worked on contemporary applications of supramolecular frameworks and adaptive chemistry with Nobel Laureate (1987) Prof. Jean-Marie Lehn at Universitè de Strasbourg (France). His research experience/interests are in the fields of (a) host-guest interactions for molecular recognition, (b) fluorescence signalling and bio-imaging, (c) metal ion detection, (d) cyto-/Phyto-toxicological assessment of bio-accumulation, (e) luminescent and colourant particles, and (f) self-healing and adaptive polymer with luminescent marker. He has 50 S.C.I. journal publications, 29 conference presentations in India and 7 presentations abroad, and has written two book chapters. Five students have been awarded PhD degree under his guidance.

Invited Lecture 6

# Low-Dimensional Semiconductors for Optoelectronic and Sensor Applications

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Abstract

Atomically thin two-dimensional layered materials such as graphene and transition metal dichalcogenides (TMDs) have opened a new and rich field with exotic properties and exciting potential applications in the "flatland". There are enormous possibilities in combining diverse 2D layered material for unique design of ultra-smart and flexible optoelectronics devices, including light-emitting diodes, photovoltaics and photodetectors. Considerable efforts have been devoted to the van der Waals hetero-integration of different 2D layered materials to form vertical superlattices via transfer of their exfoliated or as grown flakes. On the other hand, lateral heterostructure, periodic stitching of atoms in a plane, can offer exciting opportunities for engineering the formation, confinement and transport of electron, hole, exciton, and phonon at the ultimate thickness limit. These major challenges will be discussed in this talk. Recently, we reported a substantial advance that allows the direct synthesis of seamless, high-quality TMD lateral heterostructures in the chemical vapour deposition process.[1] Our novel approach offers flexibility for continuous growth of TMD based multi-junction lateral heterostructures with controlled number of atomic layers. [1-5] These TMD heterostructures are extensively characterized through Raman and Photoluminescence spectroscopy and correlated with the electrical and structural information obtained from an aberration-corrected scanning transmission electron microscope. Furthermore, we have demonstrated the room temperature photo-response and electroluminescence characteristics of these as-grown heterostructures.

The advantage of one-dimensional semiconductors such as nanowires and their arrays for the in- situ measurement of nanoscale adhesion forces from live bacteria down to pN level, and the selective detection of biomolecules such as DNA and proteins using nanowire based field effect transistor will also be highlighted. Future challenges in integrating different low-dimensional materials for optoelectronics, flexible devices and sensors will be briefly highlighted in this presentation.

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**Dr. Prasana Kumar Sahoo** is an experimental condensed matter physicist with a broad experience in the study of different low dimensional materials. He obtained PhD in Physics from Homi Bhabha National Institute (HBNI)- a grant-in-aided institute of Department of Atomic Energy, Govt. of India. He spent several years at the State University of Campinas, Brazil, University of South Florida, U.S.A., and University of Cambridge, UK, prior to holding the assistant professor position at the Materials Science Centre, I.I.T. Kharagpur. Dr. Sahoo's work covered various areas of nanomaterials that including 2D materials and heterostructures (graphene and beyond), group III-V based semiconductor nanowires and sensors. His current research focuses on the exploration and understanding of exotic 2D materials and their heterostructures which have both fundamental and wide range of technological implications for future optoelectronics. He exploits a combination of materials synthesis, hetero-structuring, spectroscopic characterization and device fabrication for physicochemical properties assessment.

Invited Lecture 7

# Nanostructured Materials for Energy Conversion and storage Applications

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Gradual rise in energy consumption, limited stock of fossil fuels; the traditional source of energy generation, coupled with environmental damage and its retrogression has laid the base for exploration of alternate source for sustainable energy conversions and storage. So, it is highly desirable to discover next-generation renewable energy devices in a clean way to replace traditional one. Electrochemical energy conversion technologies are regarded as ideal pathways to develop efficient and clean energy devices. Electrocatalytic water splitting can produce oxygen and hydrogen by the oxygen-evolution reaction (OER) and hydrogen-evolution reaction (HER), respectively. The OER has been recognized as an important half-reaction for the development of alternative energy technologies, such as electrolyzers, metal–air batteries, and regenerative fuel-cells etc. Poor catalytic performance and lower durability of OER catalyst is the main cause of low efficiency and hinders the progress of commercialization. Similarly, for HER efficient electrocatalysts are immensely required. So the overall water splitting is somewhat hindered by large overpotential for the HER and O.E.R. on most of the electrocatalyst material. Currently, precious electrocatalyst metals Pt or noble metal oxide $IrO_2$, $RuO_2$ and $IrRuO_x$ have been regarded as the most efficient electrocatalyst for HER and O.E.R. due to their superior catalytic activity. However, large-scale implementation of these precious catalysts is hindered because of their scarcity, high cost, and poor stability. Therefore, it is crucial that low-cost alternative electrocatalysts with high activity, high durability is developed to facilitate the realization of clean-energy devices.

**Dr. Bikash Kumar Jena** is serving as a Principal Scientist, Materials Chemistry Department, CSIR-Institute of Minerals and Materials Technology, Bhubaneswar. Dr. Jena has obtained his Ph. D. in Chemistry from Department of Chemistry I.I.T., Kharagpur under the supervision of Prof. C. Retna Raj. He got the opportunity to work with Prof. Bo Zhang group at University of Washington, U.S.A. as post-doctoral fellow. He visited to Technical University of Munich, Germany as visiting scientist. He has published 70 papers in international journals of high impact, 45 papers in national and international conferences, 2 patents and 6 book chapters. His work has received more than 3600 citations with h index of 31. Five Ph.D. scholars have been awarded degree under the supervision of Dr. Jena. He has delivered number of invited talks at various institutes. He bagged several awards including: Bronze Medal -The Chemical Research Society of India (CRSI) 2021, Young Scientist Award-The National Academy of Sciences, India (NASI) 2014, Young Scientist Award - Indian Society for Electro-Analytical Chemistry 2013, Young Scientist Award - Odisha Bigyan Academy 2013, CSIR Young Scientist Award 2011, Indian Science Congress -Young Scientist Award 2009, Odisha Chemical Society-Young Scientist Award 2008. He is an Associate Editor, *Journal of Nanoscience Letters,* and a member of editorial board in international journal "*ISRN Analytical Chemistry*", *"Current Catalysis" and "General Chemistry".* He has been invited to serve as a lead guest editor for Scientific World Journal. He is a reviewer of many journal papers of international repute. He has been pursuing his research activity in the field of basic as well as applied research. In particular, new and easy synthetic routes has been developed to produce metal nanoparticles, carbon-based quantum dots, nanodots, graphene, graphene-metal/metal oxide hybrid materials which are applied for a lot of promising application in energy conversion, storage sensing, biosensing, etc. Dr. Jena's work has been highlighted in India Today magazine-September 2013.

Invited Lecture 8

# Heterostructures for Hydrogen Generation

Debabrata Pradhan

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Rapid depletion of nonrenewable energy resources due to the industrial growth in the developing and developed countries poses a great risk for the future generations. In this regard, scientific community has been exploring renewable energy sources, which could satisfy the energy hungry nations. Among the renewable energy sources, water and sunlight stand at the forefront. The energy from sunshine can be utilized to break down the water molecules to produce hydrogen and oxygen. Hydrogen is a form of chemical energy that can be used as fuel in fuel cell to produce electricity in presence oxygen/air with water as the only byproduct, thus making the process completely green. However, generation of hydrogen from water under sunlight is not that simple and requires suitable catalyst. In particular, semiconductor catalyst with appropriate band gap and band edges, high absorbance ability to create enough number of electron-hole pairs and keep them separated for the required reactions are paramount among other requirements. The probability of electron-hole recombination is high with a single semiconductor, and therefore heterostructures with two different materials, either metal/semiconductor or semiconductor/ semiconductor have been found to be more promising and have been studied widely. In this lecture, I shall take a few examples of such heterostructures and their role in water-splitting reaction to generate hydrogen.

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**Dr. Debabrata Pradhan** is an Associate Professor at Materials Science Centre, I.I.T. Kharagpur. He did his Ph.D. from I.I.T. Mumbai, two years of postdoctoral research at Dept. of Physics, Tamkang University, Taiwan, and another four years at Dept. of Chemistry, Univ. of Waterloo, Canada. He has 140 international journal papers (Citations 5900, h-index 41, i10-index 111, Google Scholar), one book (Springer Publisher), two book chapters, and two Indian patents. Published papers are in several reputed journals including A.C.S. Nano, Nanoscale, Energy Env. Sci., Scientific Reports, A.C.S. Appl. Mater. & Interfaces, J. Physical Chemistry C, Langmuir, and J. Mater. Chem. He is a reviewer of several international journals including J. Am. Chem. Soc., Adv. Mater., Adv. Func. Mater., ChemSusChem, Langmuir, A.C.S. Appl. Mater. & Interfaces, J. Phys. Chem. C, Carbon, Nanoscale, Appl. Phys. Lett., J. Mater. Chem A. Research Interests of Dr. Pradhan are in the fields of nanomaterials for the energy generation and storage Seven scholars have been awarded Ph.D. degree under his guidance and Ph.D. work of 15 more are in progress. Seventeen MTech. scholars have completed their research work with him, and work of one MTech. scholar is in progress. Dr. Pradhan has won several awards. He got Adani Award for Excellence in Teaching Physical Chemistry to the B. Tech. students at IIT-Bombay (2001-2002), MRSI Medal 2019 by Materials Research Society of India in recognition of significant contributions to the field of Materials Science and Engineering, and Faculty Excellence Award 2019 by I.I.T. Kharagpur for outstanding contributions towards Teaching, Research, and Institutional Development.

Invited Lecture 9

# Self-Assembled Nano-Architectures of Bio-based Soft Materials and Their Applications

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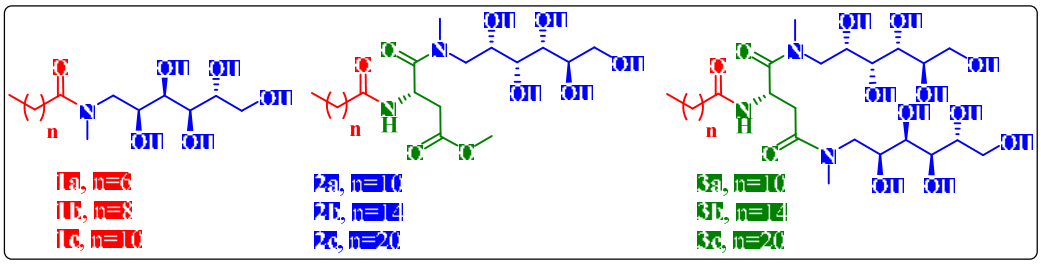
Bio-based surfactants are the green alternative to the petrochemical surfactants, which have attracted considerable interest for their industrial applications. In our laboratory three types of bio-based amphiphiles were synthesized from plant sources like vegetable oils, amino acids, and carbohydrates.

**Type 1**: Employing simple synthetic strategy glycolipid amphiphiles were synthesized and investigated for their self-assembly properties. The results show, branched nonionic surfactants molecular geometry influence the surface and micellar properties in aqueous solution. The intramolecular attractions between the highly branched headgroup lead to highly ordered micellar core ($r_{SS}$ = 0.151) with exceptionally high microviscosity of 63.7 MPa s. The orientation of chiral glucamine unit and intermolecular interactions facilitated the formation of fibrillar helical aggregates in the linear glycolipid which undergoes time dependence aggregation behavior at 25 °C. The self-assembly studies and cytotoxicity data suggests that the amphiphiles may have potential use as solubilizers and drug delivery vehicles in the pharmaceutical industry.

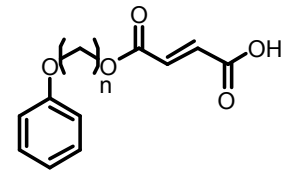


S.F.T., I.F.T., foaming, wetting, emulsification, and solubilization studies were performed as a function of glycolipid concentration. Solubilization studies provided systematic relation with increase in alkyl chain length of each glycolipid series, especially for $Y_S$ glycolipids. This indicates, with increase in hydrophobic chain length, the amphiphile activity of $Y_S$ glycolipid is more in bulk phase rather than at interface. Further, glycolipids having good foamability and foam stability exhibited chromium removal efficiency in presence of sunlight (231.3 milligram of chromium per one gram of glycolipid 3a). These glycolipids are capable to form stable emulsions with sunflower and water. Emulsification power of the glycolipids was increased with alkyl chain length and in few cases they are capable to form stable gel-emulsions. Additionally, emulsions prepared with glycolipids are able to encapsulate water and oil soluble bioactives. Obtained formulation exhibited enzyme triggered release behavior and the release rates are decreased with increase in hydrophobic chain length of glycolipids.

Further surface parameters of nine glycolipids with diverse headgroups at different hydrophobic chain lengths were studied using S.F.T. and L.B. The massive migration of surface molecules and ambiguity in limiting area per molecule of short-chain glycolipids in L.B. study was successfully reduced by addition of 5 M NaCl into water sub-phase. Overall, ST and L.B. studies are capable of providing the surface parameters of glycolipids, but each technique has its own significance and limitations. Even though the surface parameters derived from S.T. study are deviating from ideal surface behavior, but the process is spontaneous and directly reflects surfactant applications in enormous fields. The surface

parameters obtained from L.B. study provided linear structural relationship and these monolayer properties are applicable under mechanical compression only [1-5].

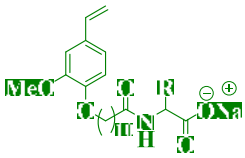
**Type 2**: Maleate based amphiphiles were synthesized using phenol, 11-bromoundecanol, and maleic anhydride as starting materials. The maleate based amphiphile entrap hydrocarbon solvents like cyclohexane, hexane, and heptane in the presence of 25 µL water, interestingly in pure solvents no gelation was observed. The dynamic mechanical strength is independent of the angular frequency ranging between 0.1 Hz to 12 Hz irrespective of the organic solvent used, though cyclohexane showed little higher magnitude in the storage modulus (G') value. The pH-induced release of vitamin $B_{12}$ from the vitamin $B_{12}$-loaded PUDMS organogel, showing potential application in pH-triggered nutraceutical release. Further a maleate based symmetric bolaamphiphile was synthesized by using cost-effective starting materials under mild reaction condition. The gelation ability of bolaamphiphile in aqueous medium was examined for a series of organic solvents. In hexane, the gelator showed better gelation ability with relatively higher critical strain (54 Pa) values. These gels showed a high internal-phase mole ratio of the topical drugs in the order of curcumin < salicylic acid < Ibuprofen. Formation of aqueous and organic gel-phase formulation may facilitate the topical medications for various applications related to ophthalmic and skin infections.




**n = 6 (6-PAM)**
**n = 8 (8-PAM)**
**n = 10 (10-PAM)**
**n = 12 (12-PAM)**

Phenoxy-alkyl maleate based amphiphiles formed stable and thermoreversibility hydrogels. Encapsulation of curcumin (1%) in the hydrophobic pockets of hydrogel was achieved. Trapped hydrophobic drug was released from gel network structure by the lipozyme enzyme. Herein, ester bond between phenoxy alkanol and maleic anhydride was hydrolysed by the enzyme. Hydrolysis of gelator molecule leads to gel degradation and subsequent release of curcumin from gel networks. In addition, when the curcumin trapped hydrogel was exposed to acidic pH, the curcumin was efficiently released within 55 min. These hydrogels may find applications as the drug carrier agent in the pharmaceutical field. Further this amphiphile showed phase-selective gelation behavior with edible oils in the biphasic mixture of oil and water. The phase selective gelation of n-PAM gelator molecules was unaffected in case of blended oils and different aqueous phases. After phase selective gelation, the edible oil can be recovered quantitatively (>95%) through simple distillation. The molecular gelators may hold future promise for remediation of an oil spill, thus reduces the environmental impact of oil spills [6-9].

**Type 3**: In an attempt to prepare bio-based green surfactant, we have synthesized vinylguaicol based anionic surfactants having polymerizable group. The detergency properties such as foaming, wetting, emulsification value and calcium tolerance were evaluated. The studied surfactants possess excellent emulsion stability and moderate calcium tolerance as compared to the commercially available surfactant SLS, Dynamic light scattering and steady state fluorescence anisotropy study were carried out to shed light on the bulk micellization properties of the synthesized surfactant. The surfactants form chiral aggregates above the critical micelle concentration as indicated by circular dichroism spectra. These surfactants may be suitable candidate as additives to detergents to improve their calcium tolerance especially in case of hard water. Further low foaming ability along with high emulsion stability may find these surfactants to be better replacement of the conventional surfactant used as emulsifier in many industrial applications [10,11].

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**Dr. Rati Ranjan Nayak** is currently working as Senior Scientist in the Department of Organic Synthesis and Process Chemistry, CSIR-IICT. obtained his Master and PhD (2002) degree from Utkal University, Odisha. He has carried out postdoctoral research work at I.I.T., Kharagpur; Kyung Hee Univrsity, South Korea; Pusan National University, South Korea and Kyoto University, Japan. He has worked as fellow scientist in the Institute of Minerals and Materials Technology (IMMT), Bhubaneswar for more than 2 years, before joining Indian Institute of Chemical Technology (IICT) in the year 2011. He has 23 years of research experience in the area of polymers, surfactant and nano- emulsions. His research mainly focuses on synthesis, characterization of surfactants (low molecular weight and polymeric); Evaluation of surface properties along with self-assembly properties of synthetic amphiphiles in aqueous solutions; Gelation behavior of low molecular weight Organo gelator and its applications. He has 55 international journal publications and 41 conference proceedings. 6 student got PhD degree under his guidance (3 as Supervisor and 3 as co-supervisor). In the year 2010, Odisha Bigyan Academy conferred Dr Nayak, young scientist award in the physical science category.

Invited Lecture 10

# Development of Nanostructured Materials for Cancer Theranostics

K. C. Barick

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Recent advances in nanobiotechnology play an important role in designing multifunctional nanostructured materials that can address the shortcomings in the area of cancer theranostics (combination of therapeutics and diagnostics). Among the others, multifunctional $Fe_3O_4$, ZnO, CuS, Au and lipid nanoparticles possess unique physio-chemical properties with an ability to get functionalized at molecular and cellular level. In general, the theranostic applications require narrow size distribution of particles and their long term colloidal and chemical stability in biological fluid. Further, significant challenges lie in avoiding undesirable uptake of these particles by reticulo-endothelial system (R.E.S.) as well as their site-specific targeting in *in-vivo* studies. Therefore, the diagnostic and therapeutic efficacy of these nanoparticles primarily depends on their design and surface engineering.

In this talk, the development of stimuli (pH, temperature, ultrasound) responsive $Fe_3O_4$, ZnO, CuS, Au and lipid based nanocarriers that are amenable for cancer theranostics will be discussed. It has been observed that surface engineering of nanoparticles allows us to create functionalized exterior with high densities of organic moieties having amine, carboxyl, hydroxyl, phosphate and sulphate functional groups for conjugation of anticancer drug molecules, receptors and fluorescent probes. Specifically, the high loading affinity of nanocarriers for anticancer drugs, their sustained release profile, self-heating capacity, low toxicity and good cellular internalization make these nanocarriers suitable for the combination therapy. Among the others, the in-house developed liposomal formulation has tremendous impact in restricting the cost of imported anticancer drug formulations. Cytotoxicity and mice model studies indicate its efficacy comparable to those available in the market. Moreover, several representative examples of multifunctional nanostructured materials having importance in drug delivery, hyperthermia and magnetic resonance imaging will be presented.

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**Dr. K. C. Barick** obtained his Ph.D. Degree in Metallurgical Engineering and Materials Science from Indian Institute of Technology Bombay, India in 2009. He was awarded prestigious DAE-BRNS KSKRA fellowship in 2010 and subsequently joined as a Scientific Officer in Chemistry Division, BARC. He was a visiting research fellow in the Department of Materials Science and Engineering at Northwestern University, U.S.A. under NSF-MWN Program. His research interest includes synthesis, surface functionalization and self-assembly of nanoscale multifunctional materials, and investigation of their potential applications in biomedical and environmental field. He has 75 publications in international journals and two patents. He has developed bioavailable nano formulation of nutraceuticals, the technology for which has been transferred to two Indian industries. He has also received DAE SSPS Young Achiever Award in 2016 and DAE Group Achievement Award in 2018.

Invited Lecture 11

# Research activity using Eggshell Particles – A low cost material with high potential applications

Sukalyan Dash

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Egg shell particles (E.S.P.) are natural substances with porous structures, which integrate various functions and have many characters superior to artificial porous structures. These materials have the same Young's modulus as steel but are much lighter. Chicken eggshells possess a highly ordered structure and comprise five structurally different layers. From the inside outwards, these include the shell membranes (inner and outer), mammillary layer, palisade layer, vertical crystal layer and cuticle (Figure 1).

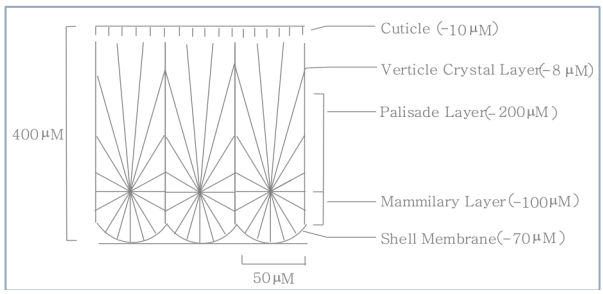


**Figure 1** Five highly ordered structurally different layers of chicken eggshell.

The eggshell is a bioceramic material, composed of approximately 95% calcium carbonate in the form of calcite and approximately 3.5% proteins, proteoglycans and glycoproteins. The organic components might be influencing nucleation, control crystal growth and shape, and play a role in determining the mechanical properties of the resulting composite. Besides calcium and carbon, the other major elements are magnesium and sodium.

Among living systems, biomineralization is a widespread phenomenon which leads to the formation of precisely controlled inorganic–organic composites, wherein the minute organic component exerts substantial control on the mineralization process resulting in the formation of particles of uniform size, novel crystal morphology, specific crystallographic orientation and interesting properties. Hence, utility of egg shell particles have been explored in the field of biomimetic design for the production of advanced composites with optimized novel properties leading to advances in materials design inspired by biological processes.

Eggshell wastes have been used as excellent bioadsorbents for the removal of various textile dyes, ecologically harmful dyes, chlorophenols, non-biodegradable metal ions, and many more such materials from water bodies around the globe. Natural Eggshell Membrane (NEM) is a new novel dietary supplement that contains naturally occurring glycosaminoglycans and proteins essential for maintaining healthy articular cartilage and the surrounding synovium. Usage of eggshell calcium has been proposed for pharmaceutical applications for calcium deficiency therapies in humans and in animals for bone mineralization and growth. A 21 kDa protein present in soluble eggshell matrix proteins plays an important role in increasing calcium transport across intestinal epithelial cells using in vitro Caco-2 cell monolayers, a type of cell cluster currently being utilized as in vitro models for absorption studies involving minerals, amino acids, protein, and peptides. Eggshell membrane possesses antibacterial

activity due to the presence of β-N-acetylglucosaminidase (β-NAGase), lysozyme, and ovotransferrin. Eggshell membrane bound enzymes are subjected to covalent coupling with a mixture of lipase, glycerol kinase and glycerol-3-phosphate oxidase to construct a triglyceride (TG) biosensor.

Egg shell waste materials have been used as the precursor of composite materials. A polypropylene composite using eggshell (ES) has been synthesized, which has a relatively lower density compared to mineral calcium carbonate with higher crystallinity. Morphological properties of composites from poly(styrene-β-ethylene/butylene-β-styrene) (SEBS) composite materials with eggshell and silk fillers are found to show good dispersion and presence of minimum large voids. Eggshell powder behaves as an excellent stabilizing material in clay related composite stuffs. Natural E.S.P. obtained from chicken eggshell have suitable properties for its use as a bone substitute in the field of maxillofacial surgery.

Eggshell particles possess catalytic usages in chemical processes. Calcined eggshell was used as an efficient and cheap catalyst to make the process of trans-esterification economic and eco-friendly, accordingly reducing its price and making it competitive with petroleum diesel. Eggshell-derived catalyst has been used to synthesize dimethyl carbonate (DMC) from the trans-esterification of propylene carbonate and methanol.

Besides the above applications, eggshell waste materials can be used as template materials, precursor for nanomaterial synthesis, precursor of calcium network synthesis and adsorption of organic substrates. Eggshell particles and membranes are an excellent source of various inorganic and bioorganic materials. Suitable processing may be developed for using them as food supplements. Since the material is abundant, low-cost, biodegradable, and has valuable applications in chemistry and chemical technology, further detailed studies on this material may propel its classification as an excellent utility material.

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**Prof. (Dr) Sukalyan Dash** is Professor of Chemistry, Veer Surendra Sai University of Technology, Burla. He passed M.Sc., M.Phil. from Sambalpur University and was awarded PhD from the same University. He has published 40 journal papers of International and national repute, such as, ACS, Elsevier, Springer, Taylor and Francis, and RSC. Five PhD scholars have been awarded degree under his guidance and six more are now working with him. He received 'Prof. R. C. Tripathy Award' and 'Prof Dayanidhi Patnaik Award' from by Orissa Chemical Society.

Invited Lecture 12

# Electrospun Polymer Nanofiber Materials: Surface Functionalization and Environmental Applications

Shabna Patel[a] and Garudadhwaj Hota[b*]

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Among many polymer nanofibers fabricating methods, electrospinning is perhaps the most versatile process. Over past few decades' nano-sized fibers of different materials such as polymer, composites, ceramic and metal oxides have been successfully fabricated using electrospinning method directly or through post-spinning processes. However, what makes electrospinning different from other nanofibers fabrication processes is its ability to form various fiber assemblies. In electrospinning process polymer nanofibers (with diameter 10 nm to 1µl) can be produced using an electrostatically driven jet of polymer solution (or polymer melt). These nanofibers produced are useful in a wealth of applications that include catalysis, composites, membrane separation, gas storage, energy conversion, tissue engineering, sensing, and environmental remediation. In this present work, we have successfully synthesized polyacrylonitrile (PAN) nanofibers by electrospinning method and have functionalized their surface with different organic molecules as well as inorganic nanoparticles. The formation, size and morphology, crystalline structure etc., of the prepared functional P.A.N. nanofibers membranes were characterized by using various analytical techniques such as FE-SEM, EDAX, TEM, XRD, FT-IR and UV-VIS. The functional PAN nanofibers membranes were used as novel nanoadsorbent materials for environmental clean-up specifically decontamination of toxic organic pollutants and also for killing harmful microorganisms from water media. Cationic and anionic dye molecules are used as model organic pollutants in this study. The obtained experimental results indicate that the functionalized electrospun nanofibers membranes were highly efficient for adsorptive removal of both cationic and anionic organic pollutants from water and also act as strong antibacterial agent against both gram positive *M. luteus* and gram-negative *E. coli* microorganisms.

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**Dr. Garudadhwaj Hota** is an Associate Professor in the Dept. of Chemistry, NIT Rourkela. In 1997 he did M.Sc. & M. Phil. In 1998 at Sambalpur University. He did Ph.D. at IIT Bombay in 2004. For postdoc he worked in National University Singapore (2004-2007). He joined NIT Rourkela as an Asst. Professor in Dept. of Chemistry (2007-2012), where is he became Associate Professor since 2012. Five Ph.D. scholars have been awarded their degree under his guidance, and six scholars are currently working. He has 45 journal publications in National & International Journals, 30 papers in conference proceedings, and six Book Chapters. The areas of research interest are nanomaterials and nanocomposites, polymer nanofibers, and functional materials for energy and environmental applications.

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