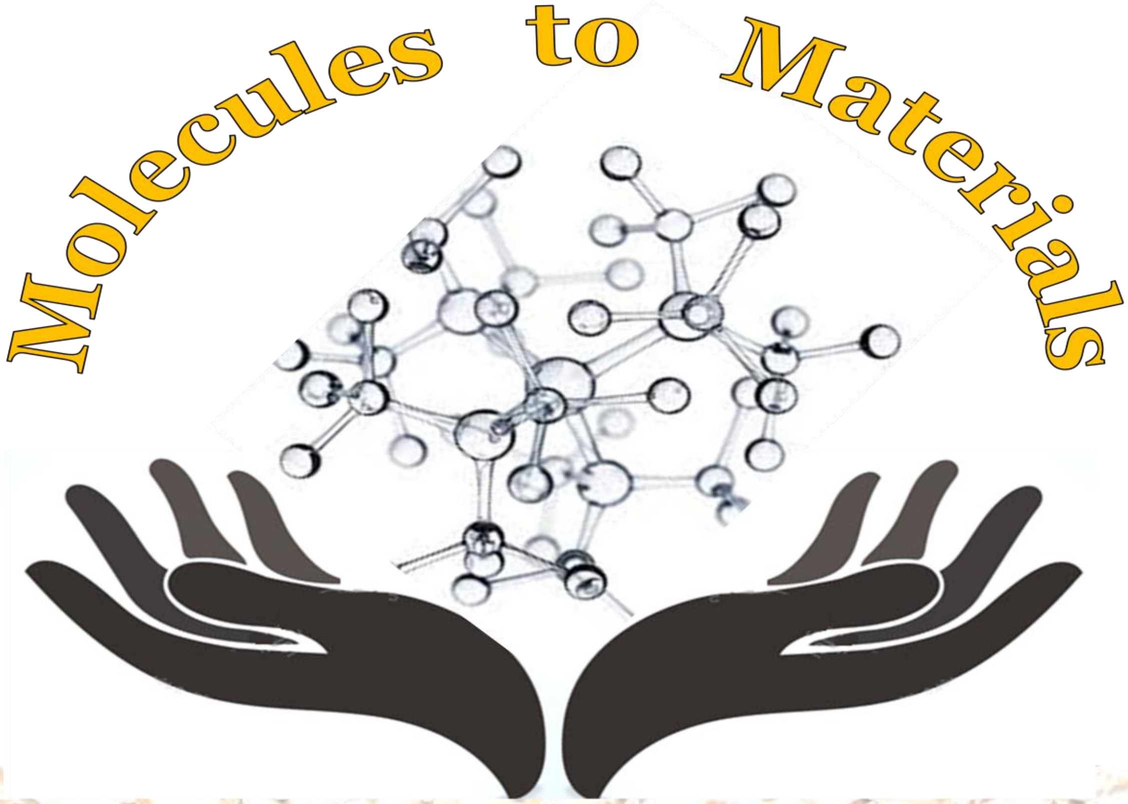
SARDAR VALLABHBHAI NATIONAL INSTITUTE OF TECHNOLOGY
SURAT-395007, GUJARAT, INDIA

Virtual
International Conference on



Molecules to Materials

MTM 2020

17-18 December 2020

Organized by
Dr. SMITA JAUHARI
Dr. KALPANA C. MAHERIA
Dr. PREMLATA KUMARI
Dr. SUBAN K. SAHOO
Dr. KETAN C. KUPERKAR

APPLIED CHEMISTRY DEPARTMENT

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ABOUT THE DEPARTMENT

The Department of Applied Chemistry came into existence in the year 1961-62. The department has 11 dedicated faculty members with the specialization in various areas. The department is running five year integrated M.Sc. including Ph.D. in various disciplines such as green chemistry, catalysis, corrosion, sensors, ion exchange, polymers, organic synthesis, natural products, drugs, dyes, supramolecular chemistry, inorganic chemistry, ionic liquids, surface chemistry, functional materials, biomaterials, nanomaterials, mass spectrometry, microchip and capillary electrophoresis and water treatment.

Mission of the Department

"The mission of the Applied Chemistry Department is to provide educational programs that would encourage students to read critically, reason analytically, communicate persuasively, apply professionally."

Vision of the Department

"The vision of the Applied Chemistry Department is to recognize itself as renowned department in the field of technical education in Applied Chemistry Department and strives to carry out the superior level of research based on the quality, innovation and excellence; with the help of its stakeholders viz. the students, research scholars, faculty members, the support staff and the alumni."

ORGANIZER’s MESSAGE

The organizing committee of Applied Chemistry Department, have an immense pleasure to welcome all the delegates of two days’ virtual international conference on ‘**Molecules to Materials – 2020**’ (MTM – 2020), at Sardar Vallabhbhai National Institute of Technology (SVNIT), Surat, Gujarat, India.

It is a matter of immense pleasure to inform that the resource persons at this conference are well-known leaders in their domain. The lectures delivered by eminent resource person, promises to be enlightening and thought provoking. The deliberations in the conference would ensure to provide the recent advancement in the fields of material science and technology and the current challenges in this domain. The aim is to inspire and encourage young research minds, which enable them to identify problems and take up new challenges covering worldwide issues such as need of advanced materials and technologies against pandemic, environment pollution etc. by gaining knowledge of ongoing current research practices in the theme areas of conference. We have provided the platform to the scientific community and policy makers, to interact and share their key research findings with the delegates across the globe.

Our sincere thanks to our Honourable Director for his immense support and guidance from the beginning. We would like to thank our Deputy Director for constant motivation and support. We would also like to thank our Head and our colleagues in the department for their constant support and efforts in creating the remarkable scientific program you are about to experience. We greatly acknowledge all the members of advisory committee for their valuable suggestions in organizing this conference.

We express our gratitude to our eminent speakers for accepting our invitation and gracing this occasion. We would also want to express my gratitude to our sponsors ACS, RSC and Chemosensors for sponsoring various awards in Young Scientist, Oral and Poster categories, which will boost the scientific wisdom in the young budding researchers.

We wish you an enjoyable, fruitful, and scientifically profitable virtual conference.

Organizing Committee
MTM - 2020
Applied Chemistry Department,
S. V. National Institute of Technology, Surat

SPONSORS AND PUBLICATIONS

ACS Publications
Most Trusted. Most Cited. Most Read.

1. ACS will give five Best Oral Presentation Awards: *The winners will get an ACS journal e-certificate and a one-year complimentary ACS Membership from the journals: ACS Omega, ACS Applied Nano Materials, ACS Applied Polymer Materials, ACS Applied Bio Materials, Langmuir*.
2. All interested participants of the conference will get a 50% discount on ACS Membership (please contact conference organizer, mtm2020svnit@gmail.com)

ROYAL SOCIETY OF CHEMISTRY

New Journal of Chemistry' will award e-certificate to the best poster.

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The journal '**Chemosensors**' is sponsoring three awards: one best poster, one oral presentation and one young scientist. All awardees will get 50% discount on one submission to chemosensors.

ELSEVIER
materialstoday: PROCEEDINGS

Participants can submit their original unpublished full paper for publication in '**Materials Today: Proceeding**'. For more details, please visit the website: Materials Today: Proceedings - Journal - Elsevier.

GENERAL INSTRUCTIONS FOR PRESENTATIONS:

(a) Please keep sufficient internet data for these two days.
(b) Mute always, while attending and when not presenting.
(c) Please keep your video Switch-ON while presenting.
(d) Join before the session begins.
(e) Attendance is important to qualify for the various awards.
(f) Please wait for your turn to upload your presentation.
(g) Please stick on to the time allotted for the presentation.
(h) Please take care of surrounding noise, while presenting.

YOUNG SCIENTIST AWARD (YSA)

For YSA presentation, please prepare your presenting materials in PPT format and present within 12 min and 3 minutes for **rigorous** discussion. **Total = 15 minutes.**

ORAL PRESENTATION

For oral presentation, please prepare your presenting materials in PPT format and present within 8 minutes and 2 min for discussion. **Total = 10 minutes.**

POSTER PRESENTATION

For poster presentation, please prepare your presenting materials in **one slide** in PPT format and present online **within 5 minutes**.

NOTE: **Follow the Indian Standard Time (IST) for all sessions.**

LINKS FOR PRESENTATIONS:

Google meet Link-1
(Inauguration, Keynote lectures and Parallel session-1)
https://meet.google.com/hin-ytup-qxi?hs=122&authuser=0

Google meet Link-2
(Parallel session-2)
https://meet.google.com/zwt-edro-rpj?hs=122&authuser=0

Google meet Link-3
(Parallel session-3)
https://meet.google.com/htp-xvgs-dtu?hs=122&authuser=0

Topic: Special Talk by Nobel laureate Prof. Jean-Marie Lehn
Time: Dec 17, 2020 06:50 PM (IST) Mumbai, Kolkata, New Delhi.

Join Zoom Meeting

https://us02web.zoom.us/j/84625449042?pwd=MnFCQW5DQXZmbU1IN0JoUTQ1cmtSUT09

Meeting ID: 846 2544 9042
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One tap mobile
+12532158782,,84625449042#,,,,,,0#,,614478# US (Tacoma)
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Passcode: 614478
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LIVE TELECAST (Youtube): https://youtu.be/wr5PIrq88l0

MTM 2020 CONFERENCE SCHEDULE

Day 1	**17th December 2020**		
IST TIME	**TECHNICAL LINE-UP**		
9:00 – 9:30	**INAUGURATION**		
9:30-11:40	**KEYNOTE Lectures**		
	Session Chair(s): Dr. Ketan Kuperkar and Dr. Smita Jauhari		
9:30-10:10	**KN– 01**	**Prof. A. K. Mishra, IIT Madras.**	
10:10-10:50	**KN – 02**	**Prof. Shin-ichi Yusa, University of Hyogo, Japan.**	
10.50-11:30	**KN – 03**	**Prof. Kuruvilla, IIST, Thiruvanathapuram.**	
11:40-1:30	**INVITED Lectures and Oral Presentations**		
	Parallel Session-I	**Parallel Session-II**	**Parallel Session-III**
	Session Chair: **Dr. Dhreeraj Singh, IITRAM**	**Session Chair:** **Dr. Sanjay Tiwari, UTU**	**Session Chair:** **Dr. R. K. Joshi, MNIT Jaipur**
11:40-12.10	**IL-01 Prof. S. Velmati, NIT Trichy, Tiruchirappalli.**	**IL-02 Prof. N. V. Sastry, Sardar Patel University, Gujarat.**	**IL-03 Prof. Sriram, IIT, Gandhinagar.**
12.10-12.20	OP-1 Shah Jaimin Balkrishna, Government Commerce and Science College, Gujarat.	OP-9 Vinod Kumar, SVNIT, Gujarat.	OP-17 Geeti Kaberi Dutta, Tezpur University, Assam.
12.20-12.30	OP-2 P. Karuppusamy, VIT, Vellore.	OP-10 Chetan R. Patel, PPSU, Gujarat.	OP-18 Abhishek A. Gor, Nirma University, Gujarat.
12.30-12.40	OP-3 Hemant P. Soni, MSU, Gujarat.	OP-11 Sadafara A. Pillai, PPSU, Gujarat.	OP-19 Sakshi, NIT Jalandhar.
12.40-12.50	OP-4 Mujthaba Aatif A, VIT, Vellore.	OP-12 Bratin Kumar Das, NIT Mangalore.	OP-20 Amita Chaudhary, Nirma University, Gujarat.
12.50 -1.00	OP-5 Patitapaban Mohanty, Veer Surendra Sai University of Technology Burla, Odisha.	OP-13 Sonal Thakore, MSU, Gujarat.	OP-21 Dipti D. Parmar, Gujarat University, Gujarat.
1.00-1.10	OP-6 Natarajan Vijay, NIT Tiruchirappalli.	OP-14 Shehnaz H Solanki, Navarachana University, Gujarat.	OP-22 Zakiullah Zaidi, NIT Nagpur.
1.10-1.20	OP-7 Anusuyadevi Kathiresan, NIT Trichy.	OP-15 Mitali Dugvekar, NIT Bhopal.	OP-23 Sonil Nanda, University of Saskatchewan, Canada.
1.20-1.30	OP-8 Sunita Behera, Veer SurendraSai University of Technology Burla, Odisha.	OP-16 Dimpee Sarmah, Tezpur University, Assam.	OP-24 Falguni T. Patel, Navyug Science College, Gujarat.
LUNCH BREAK			

2:00 – 3:20	**KEYNOTE LECTURES**		
	Session Chair: Dr. Suban K Sahoo and Dr. Premlata Kumari		
2:00 – 2.40	**KN–04 Professor Run, The University of Queensland, Australia**		
2:40 – 3:20	**KN –05 Prof. Y. Bao, Department of Chemistry and Applied Biosciences, Switzerland**		
3:20-6:00	**INVITED Lectures and ORAL Presentations**		
	Parallel Session-I	**Parallel Session-II**	**Parallel Session-III**
3:30-6:00	**Session Chair: Dr. Dhiraj Bhatia**	**Session Chair: Prof. M. Mukhopadhyay**	**Session Chair: Prof. M. Chakraborty**
3.20-3.50	**IL-04 Prof. N. Singh, Indian Institute of Technology Ropar, Rupnagar.**	**IL-06 Dr. V. K. Gupta, Reliance Industries Limited, Navi Mumbai.**	**IL-08 Prof. S. C. Moi, NIT Durgapur, West Bengal.**
3.50-4.20	**IL-05 Prof. P. C. Mondol, IIT Kanpur, Kanpur.**	**IL-07 Dr. Dhreeraj Singh, IITRAM, Ahmedabad.**	**IL-09 Dr. Indrajit Shown, Amrita Vishwa Vidyapeetham, Kochi.**
4.20-4.30	OP-25 Arpita S. Desai, MSU, Gujarat.	OP-35 Ruchi Sharma, IIT Roorkee.	OP-45 Seshu Vardhan, SVNIT, Gujarat.
4.30-4.40	OP-26 K.C. Pradhan, Utkal University, Odisha.	OP-36 Asna Mariyam, NIT Bhopal.	OP-46 Kunj S Talati, Uka Tarsadia University, Gujarat.
4.40-4.50	OP-27 Mayuri Shaiwale, MSU, Gujarat.	OP-37 Paritosh Agnihotri, SVNIT, Gujarat	OP-47 Amar Deshamukh, Uka Tarsadia University, Gujarat.
4.50-5.00	OP-28 Susital Mal, NIT Patna.	OP-38 Devappa S. Lamani, Rani Channamma University, Karnataka.	OP-48 Hemanshu Patel, MSU, Gujarat.
5.00-5.10	OP-29 Tarushyam Mukherjee, IIT Gandhinagar.	OP-39 Satya Ranjan Jena, IISER Bhopal.	OP-49 Anuj K Saini, SVNIT, Gujarat.
5.10-5.20	OP-30 Mini Loya, NIT Arunachal Pradesh.	OP-40 Aswathy Chandra.Y.C, Noorul Islam Centre for Higher Education, Tamilnadu.	OP-50 Hem N. Naik, SVNIT, Gujarat.
5.20-5.30	OP-31 Shilpa Sharma, IIT Rupnagar.	OP-41 Sanjiv O. Tomer, MSU, Gujarat.	OP-51 Dilip C. Kanjariya, SVNIT, Gujarat.
5.30-5.40	OP-32 Umme Solaem Akond, Aasam University, Aasam.	OP-42 Uplabdhi Tyagi, Guru Gobind Singh Indraprastha University, New Delhi.	OP-52 Alivia Mukherjee, University of Saskatchewan, Canada.
5.40-5.50	OP-33 Pravin Kumar Selvam, VIT Vellore.	OP-43 Keshavi Nalla, University of Hyderabad, Telangana.	OP-53 Kingsuk Mahata, IIT Guwahati, Assam.
5.50-6.00	OP-34 Salma Mitchla, VNSGU, Gujarat.	OP-44 Sameer Maurya, NIT Jalandhar	OP-54 Madhu Bala, NIT Jalandhar.
A SPECIAL TALK BY NOBEL LAUREATE – Professor Jean-Marie Lehn			
7:00- 8:00	**From Supramolecular Towards Adaptive Chemistry Towards Functional Dynamic and Adaptive Materials**		

Day 2	**18th December 2020**		
IST TIME	**TECHNICAL LINE-UP**		
9:00-11:00	**KEYNOTE Lectures**		
	Session Chair: Dr. Kalpana Maheria and Dr. Smita Jauhari		
9:00 – 9:40	**KN– 06**	**Prof. Ajay Dalai, University of Saskatchewan, Canada**	
9:40-10:20	**KN – 07**	**Prof. Q. Su, Shanghai University, Shanghai**	
10:20-11:00	**KN – 08**	**Professor Chae, Hanyang University, South Korea**	
11:00-12:00	**YOUNG SCIENTIST AWARD Lectures**		
	Session Chair: Prof. Sriram, IIT Ganghinagar		
11.00-11.15	YSA-01	Rajamouli Boddula, Uka Tarsadia University, Gujarat.	
11.15-11.30	YSA-02	Bigyan R. Jali, Odisha.	
11.30-11.45	YSA-03	Dhruvi Patel, SVNIT, Gujarat.	
11.45-12.00	YSA-04	Radha N Somaiya, SVNIT, Gujarat.	
12:00-1:55	**INVITED Lectures and ORAL Presentations**		
	Parallel Session-I	**Parallel Session-II**	**Parallel Session-III**
	Session Chair: Dr. A K Mungray	**Session Chair: Prof. Kashinath Durke**	**Session Chair: Dr. Sanjay Patel**
12.00-12.25	**IL-10 Prof. Ashok S. K., Vellore Institute of Technology, Vellore.**	**IL-13 Dr. Dhiraj Bhatia, IIT Gandhinagar.**	**IL-16 Dr. Vijay Narkhede, Süd Chemie India (P) Ltd, Vadodara.**
12..25-12.50	**IL-11 Dr. Anant Atta, NIT Arunachal Pradesh.**	**IL-14 Prof. Sanjay Tiwari, UKA Tarsadia University, Gujarat.**	**IL-17 Dr. M. A. Shah, NIT Srinagar.**
12.50-1.15	**IL-12 Prof. V. K. Jain, Raipur Chhattisgarh.**	**IL-15 Dr. R. K. Joshi, MNIT Jaipur.**	**IL-18 Prof. Pankaj Kandwal, NIT Srinagar.**
1.15-1.25	OP-55 A. Singh, Chandigarh University, Mohali.	OP-59 Aayushi Lodhi, SVNIT, Gujarat.	OP-63 Dipesh D. Kachhadiya, SVNIT, Gujarat.
1.25-1.35	OP-56 D. Sharma, SVNIT, Gujarat.	OP-60 Anil Kumar Jangir, SVNIT, Gujarat.	OP-64 S. Morang, Tezpur University, Assam.
1.35-1.45	OP-57 Sowmyashree A S, Presidency University, Bangalore.	OP-61 Hina N. Chaudhari, Gujarat University, Gujarat.	OP-65 Ranjan Kumar Padhy, NIST, Orissa.
1.45-1.55	OP-58 Sk Arif Mohammad, IIT Bhilai.	OP-62 Biswajit G. Roy, Sikkim University, Sikkim.	OP-66 Girish Kamath, University of Saskatchewan, Canada.
LUNCH BREAK			

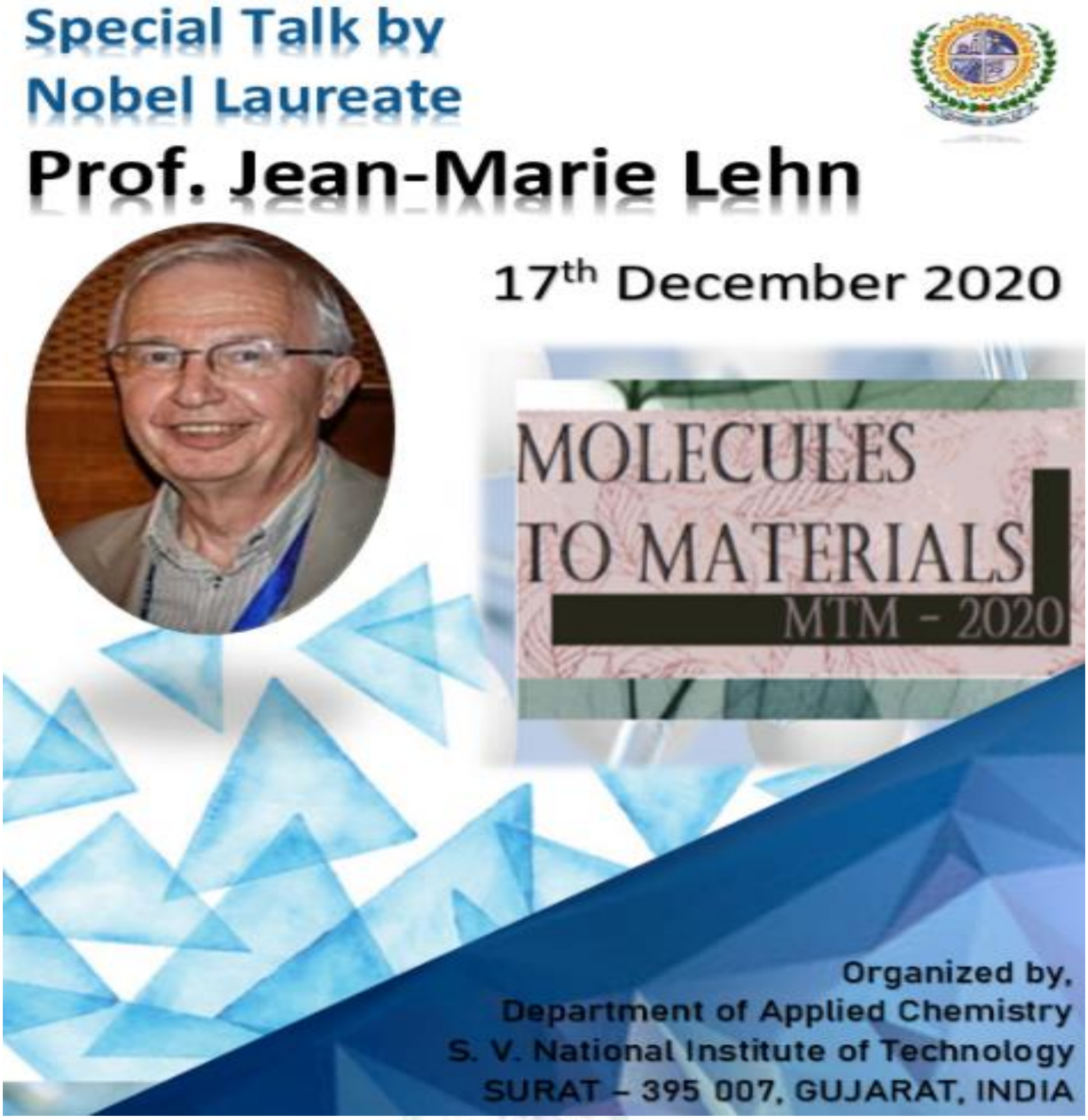
2:20-3:40	**KEYNOTE Lectures**	
	Session Chair: Dr. Premlata Kumari and Dr. Ketan Kuperkar	
2:20 – 3:00	**KN–09**	**Prof. Gopinath Sankar, University College London, UK**
3:00-3:40	**KN –10**	**Prof. Reza, Sharif University of Technology, Iran**

3:40-4:55	**YOUNG SCIENTIST AWARD Lectures**	
	Session Chair: Prof. Sriram, IIT Ganghinagar	
3.40-3.55	YSA-05	Jyotsnamayee Nayak, SVNIT, Gujarat.
3.55-4.10	YSA-06	Dhara Morawala, SVNIT, Gujarat.
4.10-4.25	YSA-07	Vinita Bhardwaj, SVNIT, Gujarat.
4.25-4.40	YSA-08	Azazahemad A. Kureshi, SVNIT, Gujarat.
4.40-4.55	YSA-09	Riddhi Joshi, Maharaja Krishnakumarsinhji Bhavnagar University, Gujarat.

5:00 – 7.00	**INVITED Lectures and POSTERS Presentations**		
	Parallel Session-I	**Parallel Session-II**	**Parallel Session-III**
	Session Chair: Dr. Y. Sonwane	**Session Chair: Dr. Jyoti Meghani**	**Session Chair: Dr. Dimple Shah**
5.00-5.30	**IL-19 Prof. Lee Wilson, University of Saskatchewan, Canada.**	**IL-21 Prof. Raj Kamal, Kurukshetra Uni., Haryana.**	**IL-22 Dr. Sonil Nanda, University of Saskatchewan, Canada.**
5.30-6.00	**IL-20 Prof. Kashinath Dhurke, NIT, Warangal**	**IL-23 Prof. Y. C. Sharma, IIT, BHU**	-
6.00-7.00	PP-1 Dr. G. Dilli Rani, Bapatla Women's Engineering College, Andhra Pradesh.	PP-13 Falguni Shukla, MSU, Gujarat.	PP-25 Chitralekha Chakrabarti, PPSU, Gujarat.
	PP-2 Dr. Thangaraj Anand, Apollo Arts and Science College, Chennai.	PP-14 Hitendra A Mali, Gujarat University, Gujarat.	PP-26 Sharwan K Dewan, M D University, Rohtak.
	PP-3 Saravanakumar Manickam, VIT Vellore.	PP-15 Inimfon A. Udoetok, University of Saskatchewan, Canada.	PP-27 Divya Patel, SVNIT, Gujarat.
	PP-4 Jegathalaprathaban Rajesh, K. Ramakrishnan College of Technology, Tiruchirappalli.	PP-16 Sandeep Veda Narayana. M.S, JNTUK, Andhra Pradesh.	PP-28 Ramanjit Kaur, NIT Punjab.
	PP-5 Angana Pan, NIT Durgapur.	PP-17 Sourav De, VIT Vellore.	PP-29 Nital R. Panchal, M. G. Science Institute, Gujarat.

	PP-6 R. Bhaskar, VIT Vellore.	PP-18 Moturi Anuraag, Uka Tarsadia University, Gujarat.	PP-30 Omkar Singh, NITK, Mangaluru.
	PP-7 Satyanarayan Pal, Utkal University, Odisha.	PP-19 Abdalla H. Karoyo, University of Saskatchewan, Canada.	PP-31 Rahul Patil, Uka Tarsadia University, Gujarat.
	PP-8 Rituparna Bhaduri, NIT Durgapur.	PP-20 Henilkumar Lankapati, SVNIT, Gujarat.	PP-32 Kanchna Bhatrola, NIT Jalandhar.
	PP-9 Rubi Behura, Veer SurendraSai University of Technology Burla, Odisha.	PP-21 Khushboo D. Bhanderi, MSU, Gujarat.	PP-33 Sachin Rathod, Uka Tarsadia University, Gujarat.
	PP-10 Saikat Mandal, NIT Durgapur.	PP-22 Venu Babu Borugadda, University of Saskatchewan, Canada.	PP-34 Bharatkumar Kanoje, PPSU, Gujarat.
	PP-11 Nishith A Chudasama, CSIR-Bhavnagar, Gujarat.	PP-23 Disha Aherrao, Lovely Professional University, Punjab.	PP-35 Priyajit Jash, IIT Kanpur.
	PP-12 C. Kalaivanan, K. Ramakrishnan College of Technology, Tiruchirapalli.	PP-24 Ayushi Patel, Gujarat University, Gujarat.	PP-36 N C Kothiyal, NIT Punjab.
	-		PP-37 Tanuj Gupta, Nirma University, Gujarat.
	-		PP-38 Ajaya Kumar Behera, Utkal University, Bhubaneswar.
	-		PP-39 Abhilasha Chauhan, IIT Roorkee.
	-		PP-40 Dr. Yogesh B Wagh, KBCNM University, Jalgaon.
Valedictory Function (7.15 pm)			

TABLE OF CONTENT



Special Talk by
Nobel Laureate
Prof. Jean-Marie Lehn

17th December 2020

MOLECULES
TO MATERIALS
MTM - 2020

Organized by,
Department of Applied Chemistry
S. V. National Institute of Technology
SURAT – 395 007, GUJARAT, INDIA

Jean-Marie Lehn (born 30 September 1939) is a French chemist. He received the Nobel Prize in Chemistry together with Donald Cram and Charles Pedersen in 1987 for his synthesis of Cryptands. Lehn was an early innovator in the field of Supramolecular Chemistry, i.e., the chemistry of host-guest molecular assemblies created by intermolecular interactions, and continues to innovate in this field.

NL-01

From Supramolecular Towards Adaptive Chemistry Towards Functional Dynamic and Adaptive Materials

Jean-Marie Lehn

ISIS, Université de Strasbourg, France

Supramolecular chemistry is intrinsically a *dynamic chemistry* in view of the lability of the non-covalent interactions connecting the molecular components of a supramolecular entity and its resulting ability to exchange components. Similarly, dynamic covalent chemistry concerns molecular entities containing covalent bonds that may form and break reversibility, so as to allow a continuous modification in constitution by reorganization and exchange of building blocks. These features define a *Constitutional Dynamic Chemistry* (CDC) on both the molecular and supramolecular levels.

One may define *constitutional dynamic materials*, as materials whose components are linked through reversible covalent or non-covalent connections and which may thus undergo constitutional variation, i.e. change in constitution by assembly/deassembly processes in a given set of conditions. Because of their intrinsic ability to exchange, incorporate and rearrange their components, they may in principle select them in response to external stimuli or environmental factors and therefore behave as *adaptive materials* of either molecular or supramolecular nature.

Applying these considerations to polymer chemistry leads to the definition of *constitutionally dynamic polymers*, DYNAMERS, of both molecular and supramolecular types, possessing the capacity of adaptation by association/growth/dissociation sequences. *Supramolecular materials*, in particular *supramolecular polymers* may be generated by the polyassociation of components/monomers interconnected through complementary recognition groups. *Dynamic covalent polymers* result from polycondensation via reversible chemical reactions. They may undergo modifications of their properties (mechanical, optical, etc.) via incorporation, exchange and recombination of their monomeric components. . These features give access to higher levels of behavior such as healing and adaptability in response to external stimuli (heat, light, medium, chemical additives, etc.).

CDC introduces a paradigm shift into the chemistry of materials and opens new perspectives in materials science. A rich variety of novel architectures, processes and properties may be expected to result from the blending of supramolecular and molecular dynamic chemistry with materials chemistry, opening perspectives towards *adaptive materials and technologies*.

References

1. J.-M. Lehn, Dynamic combinatorial chemistry and virtual combinatorial libraries, Chem. Eur. J., **1999**, 5, 2455.
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5. J.-M. Lehn, "Dynamers: From Supramolecular Polymers to Adaptive Dynamic Polymers", in Adv. Polym. Sci., **2013**, 261, 155-172.
6. Lehn, J.-M., Perspectives in Chemistry – Steps towards Complex Matter, Angew. Chem. Int. Ed., **2013**, 52, 2836-2850.
7. Lehn, J.-M., Perspectives in Chemistry – Aspects of Adaptive Chemistry and Materials, Angew. Chem. Int. Ed., **2015**, 54, 3276-3289.

KN-01

White Light Emission and Mechano-fluorochromism of Acetylene Conjugated Organic Molecular Solids

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Extended conjugated chromophoric compounds containing acetylenic linkage have been of renewed current interest [1]. We have been looking in to the basic photophysics of such molecules in recent times. The butadiynyl derivatives exhibit emissions from both locally excited (LE) and ICT states in non-aqueous media [2]. The LE emission is confined to the normal mode involving C-C triple bond stretching of the butadiyne moiety. The fluorophores are twisted and the diyne moiety deviates from the usual linearity (sp) in the ICT state [3]. The diphenylbutadiynes with an acceptor group at meta position of the phenyl ring show the lowest absorption energy compared to their ortho and para isomers, which is related to the 'meta effect' well-known in organic photochemical reaction [4]. Butadiyne bridged pyrene-phenyl hybrid derivatives show LE emission originating from the pyrene moiety, which is in contrast to the observation of the LE emission in the diphenylbutadiynes [5]. The emission behavior of these molecules in their aggregate states as well as in solid states has been quite interesting. We observed emission in solid powder form, with some of the diynes showing reversible fluorescence switching in the solids. The solid state emission of the derivatives is either blue (excitonic coupling) or red (excimeric coupling) shifted with regard to the solution phase emission spectrum, depending on the bulkiness of the peripheral aromatic moiety [6]. Butadiynyl fluorophores containing donor and acceptor peripheries exhibit single component white light emission, which was exploited to polar aprotic vapor detection in a polymer film matrix [7]. We have also studied the photophysical insights of a diyne bridged classical donor-acceptor electronic energy pair, naphthalene-pyrene, in comparison with its part molecular structures [8]. Building on these studies, we further investigated the photophysics of a less explored class of cross-conjugated Y-shaped enediyne- (one double and two triple bonds) bridged organic fluorophores. These fluorophores showed interesting photophysical properties including dual emissions from locally excited (LE) and intramolecular charge transfer (ICT) states; and ring size dependent aggregate fluorescence in non-aqueous media. The enediynyl derivatives were also prone to undergo photoreactions upon continuous photon illumination, which were successfully utilized to achieve high-contrast fluorescence color switching [10]. The intriguing photophysical outcomes of the fluorophores were further exploited to generate single-component white light emission [9] and monitor micro-heterogeneity in biologically relevant anisotropic media [11].

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KN-02

Biocompatible Polyion Complex (PIC) Aggregates Formed by Electrostatic Interactions in Water

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A pair of oppositely charged diblock copolymers, poly(2-(methacryloyloxy)ethyl phosphorylcholine)-*block*-poly((3-(methacryloylamino)propyl)trimethylammonium chloride) (PMPC-b-PMAPTAC) and poly(2-(methacryloyloxy)ethyl phosphorylcholine)-block-poly(sodium 2-(acrylamido)-2-methylpropanesulfonate) (PMPC-*b*-PAMPS), was prepared via reversible addition–fragmentation chain transfer radical polymerization using a PMPC-based macro chain transfer agent[1-5]. The pendant phosphorylcholine group in the hydrophilic PMPC block has anionic phosphate and cationic quaternary amino groups, which are neutralized within the pendant group. Therefore, the mixing of aqueous solutions of PMPC-*b*-PMAPTAC and PMPC-b-PAMPS leads to the spontaneous formation of simple core–shell spherical polyion complex (PIC) micelles comprising of a segregated PIC core and PMPC shells. The PIC micelles were characterized using ^{1}H NMR spin–spin (T_2) and spin–lattice relaxation times (T_1), diffusion-ordered NMR spectroscopy, static light scattering, dynamic light scattering (DLS), and transmission electron microscopy techniques. The hydrodynamic size of the PIC micelle depended on the mixing ratio of PMPC-*b*-PMAPTAC and PMPC-*b*-PAMPS; the maximum size occurred at the mixing ratio yielding stoichiometric charge neutralization. Exchange of block copolymers (unimers) between PIC micelles due to dynamic properties of the micelles was confirmed by DLS. The PIC micelles disintegrated to become unimers with the addition of salts.

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KN-03

Surface Engineered Nanosystems for Bio-Medical and Space Applications

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In the field of medicine, its applications are not less than a magic. The availability of more durable and better prosthetics and new drug-delivery systems are of great scientific interest and give hope for cancer treatment and minimum invasive treatments for heart disease, diabetes and other diseases. One of the most promising societal impacts of nanotechnology is in the area of nanomedicine. Personalized health care, rational drug design, and targeted drug delivery are some of the benefits of a nanomedicine based approach to therapy. The most promising areas of nanomedicine are diagnostics by in vitro imaging and cancer therapies in ovarian cancer by the use of nanoparticles. New approach is its use as therapeutics modalities for infertility. Nanotechnology will serve as multifunctional tools that will not only be used with any number of diagnostic and therapeutic agents, but will change the very foundations of cancer diagnosis, treatment, and prevention. Nanotechnology is applied to the field of cancer in the development of nanovectors, which can be loaded with drugs or imaging agents and then targeted to tumours. Combined technologies can be used for both earlier diagnosis and better treatment for patients with cancer. Nanotechnology is poised to have an increasing impact on cardiovascular health in coming years. Drug delivery will be impacted by targeting of nanoparticles encapsulated drugs to the site of action, increasing the effective concentration and decreasing systemic dosage and side effects. Nanotechnologies and micro technologies can be merged with biomaterials to generate scaffolds for tissue engineering that can maintain and regulate cell behavior. Also, such technologies can be used to regulate in vitro cellular microenvironment to direct stem cell differentiation. Recent developments in the use of nanotechnologies with stem cells have been motivated by the continuous introduction of novel nanotechnology multidisclipency platforms during the last few years.

The mechanical and thermal properties of polymers and composite structures can be altered through the use of various kinds of fillers. The dimensions of these fillers typically fall on a macroscopic (1 mm^{-1} mm) length scale. However, macroscopic fillers usually cause decreases in strength, impact resistance and processability. A new area of composites research has emerged in the last two decades that utilizes nanoparticle fillers to alter the properties of polymers. Nano particle fillers can increase the modulus, strength, toughness, resistance to chemical attack, gas impermeability, resistance to thermal degradation, and dimensional stability of polymeric materials. Carbon nanotubes, nano silica, nano clay, POSS etc., are extensively used as reinforcing agents in nanocomposites. The major difficulty in optimizing composite properties with nano reinforcing agent is achieving sufficient dispersion in the epoxy matrix. The difficulty in achieving good dispersion of CNT is resolved by proper functionalization of the nano tubes. By judiciously selecting the modifier and grafting with nano reinforcing agent, we can improve the compatibility with matrix and thereby tailor the material for specific applications.

KN – 04

Responsive Probes for Background-free Luminescence Bioassay and Imaging

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Fluorescence bioassay using responsive probes has been widely used in biomedical research and pre-/clinical investigations. The development of reliable bioanalytical probes for selective and sensitive detection of particular biomolecule in biological systems plays key roles in fluorescence bioassay and is essential for better understanding the roles of the biomolecule in their native contexts. In the last two decades, a large number of fluorescence probes have been developed for the detection of biomolecules in vitro and in vivo, while it remains challenging to use these probes for biomolecules detection in the samples with high background autofluorescence signals. In this presentation, I will introduce our recent contributions to the development of responsive probes for background-free luminescence bioassay and imaging. Specifically, responsive metal complex probes with long-lifetime emission for time-gated luminescence (TGL) analysis and imaging of biomolecules in vitro and in vivo will be discussed.

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KN – 05

Digital Light 3D Printing of Biodegradable Photopolymers with Tunable Elastomeric Properties

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Additive manufacturing (commonly called 3D printing) has attracted great attention due to its powerful ability to create complex 3D geometries with precise microarchitectures. In combination with medical imaging techniques, it might provide enormous opportunities to design customized drug formulations and biomedical devices.[1] Among the existing 3D printing techniques, digital light processing (DLP) emerged with high resolution and surface quality, desktop size, designable materials and relatively low cost, which is based on a localized light-initiated photopolymerization process, taking place in a bath containing liquid (macro) monomers and photoinitiators. However, the lack of biocompatible and biodegradable materials suitable for DLP limits their application in the biomedical area, especially for the manufacture of elastic personalized devices.[2] We recently developed novel synthetic strategies to enable the digital light 3D printing of biodegradable elastomers with tunable mechanical properties.[3,4] These works open new perspectives for fabricating precise personalized medical devices with biodegradability as well as ideal elastomeric properties by 3D printing.

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KN – 06

Growth of Bioprocessing Technologies for Clean Sustainable Energy Production

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Biofuels are gaining attention as renewable energy sources to address the rising energy demands, fluctuating crude oil prices and greenhouse emissions from fossil fuels. Biofuels can be produced from a wide variety of renewable feedstocks and biogenic wastes through thermochemical, biological and hybrid conversion technologies. This presentation will highlight the candidacy of a variety of bioprocessing technologies for a wide range of waste feedstocks such as lignocellulosic biomass (e.g. agricultural crop residues and woody biomass), energy crops, sewage sludge, municipal solid waste, food waste, waste cooking oil, waste tires as well as petroleum residues (e.g. heavy/ light gas oils, bitumen, asphaltene and petroleum coke) to produce clean sustainable energy production. Although these waste residues are available in considerable amounts worldwide, their potential for resource recovery is least realized. This presentation will highlight some notable research studies conducted in the Catalysis and Chemical Reaction Engineering Laboratories (CCREL) over the past 25+ years at the University of Saskatchewan on biomass-to-gas (BTG) and biomass-to-liquid (BTL) conversion technologies to produce synthetic transportation fuels and carbon-rich solid products. The potential and performance of integrated clean technologies, especially hydrothermal gasification, liquefaction, pyrolysis and Fischer-Tropsch synthesis will be discussed along with the upgrading of biocrude oils through catalytic hydrotreating. Synchrotron-based advanced structural chemistry studies on the synthesis, characterization and application of novel catalysts and nano-catalysts used in BTG and BTL technologies will be comprehended. The current progress, challenges and knowledge gaps in the R&D of BTG and BTL technologies for the production of synthetic hydrocarbon fuels from waste resources as well as their opportunities to Canadian bio-economy will be comprehensively reviewed.

KN – 07

Design and Optical Studies of Upconversion Materials for Bioapplications

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Upconversion materials that convert low energy excitation wavelength to high energy emission have attracted considerable attention due to the advantages of high penetration depth and high resistance to autofluorescence interference capability. We present rational designs and synthesis of upconversion luminescent materials displaying unprecedented optical properties. We also demonstrate the molecular upconversion luminescent probe, which shows excellent photostability, high quantum yield and rapid excretion capability. The NIR-to-NIR upconversion technique also offers a promising detection method, which shows very high sensitivity and selectivity for the detection of Cu^{2+} ions in vitro and in vivo. In addition, the toxicity of anti-Stokes luminescent materials will be included.

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KN – 08

New Amphiphiles for Membrane Protein Structure Study: Importance of Pendant Chain in Protein Stabilization

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Membrane proteins play critical roles in a variety of cellular processes and thus are main drug targets. Structural information on membrane proteins facilitates drug discovery, but it is challenging to determine high resolution structures of these membrane-associated biomacromolecules. Amphiphilic agents called detergents are widely used for membrane protein structural study, but conventional detergents have limited ability to stabilize membrane proteins. Thus, it is necessary to develop new detergents with enhanced efficacy for membrane protein stabilization. This presentation introduces the recent inventions of novel detergents and discusses detergent design principles focusing on the roles of detergent pendant chains in membrane protein stabilization. Despite the small size compared to the whole molecule, a pendant chain can dramatically change detergent property, conferring enhanced stabilization to membrane proteins.

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KN – 09

Molecular systems as precursors for heterogeneous catalysts

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Catalysis is the back-bone of chemical industries and they will continue to be essential in numerous applications that are indispensable to enhance quality of our life and society. Several types of heterogeneous catalysts, for example, supported catalysts, bulk oxides and nanoporous materials, are widely used for a variety of catalytic reactions. Within the family of heterogeneous catalytic systems, nanoporous materials (see figure 1) are highly effective for performing shape selective reactions and hence studied widely for a variety of catalytic applications. Similarly nano sized metals and metal oxides are becoming increasingly important in a range of catalytic applications.

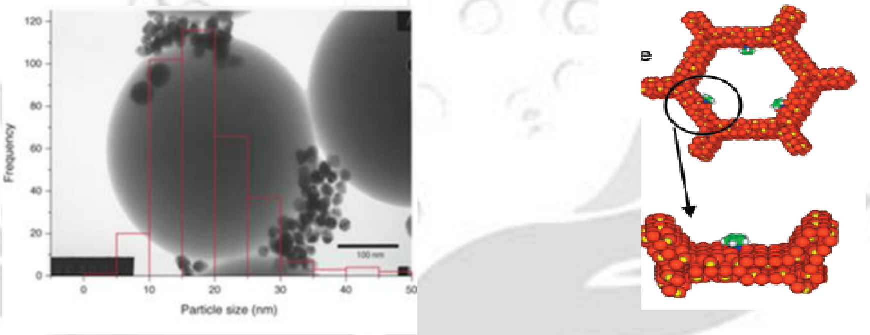

Figure 1. Typical (left) supported metal catalysts derived using molecular precursor and on right adsorbed molecular precursor on mesoporous silica are shown here.

Majority of these supported catalysts are widely used and produced using solution processing methods, specifically impregnation or co-precipitation or deposition precipitation methods. While these materials are widely used for a range of applications, use of well-defined molecular precursors of the active component to the support material could be advantageous. Here titanium supported mesoporous silica employed for epoxidation reaction, bimetallic catalyst supported on mesoporous silica for hydrogenation reaction and gold based molecular clusters supported on nano spheres of silica for oxidation of benzyl alcohol will be given as example to demonstrate the application of these preparation methods.

KN-10

Nature inspired plasmonic sensor arrays

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Array-based sensing has been inspired from nature's use of arrays of receptors in the senses of taste and smell. In this so-called "chemical tongue/ nose", each receptor (sensing element) has a semi-selective response to a particular analyte and the specificity of the sensor is accomplished by pattern-based recognition from which distinct response patterns are attained for each analyte [1]. In contrast to the lock-and-key sensing mode which demands highly specific receptors for the detection of each analyte, the sensing elements within array-based probes may have different responses towards different analytes. In other words, in the array strategy, a group of responses are collected from semi-selective sensor elements which produce a distinct pattern for the identification and discrimination of several analytes. Simultaneous determination of various analytes, especially analytes with extremely similar-looking chemical structures, becomes more important when critical decisions have to made, for instance, in the treatment of diseases, food/ drug quality control, pollution issues, criminal investigations, explosive detections and many other medical, environmental, industrial, and security concerns. In such cases, employing the unique optical features of plasmonic nanoparticles within the differential array-based sensing approach, allows the development of simple, rapid and sensitive nanostructured sensor arrays, capable of effective recognition and discrimination of groups of target species [2-5].

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IL-01

Development of Sensors for endogenous detection of Reactive Oxygen, Sulphur Species and Hydrazine

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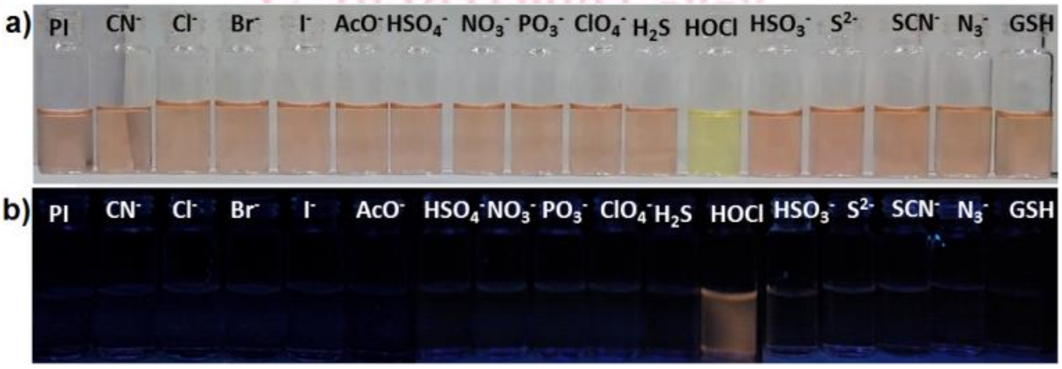
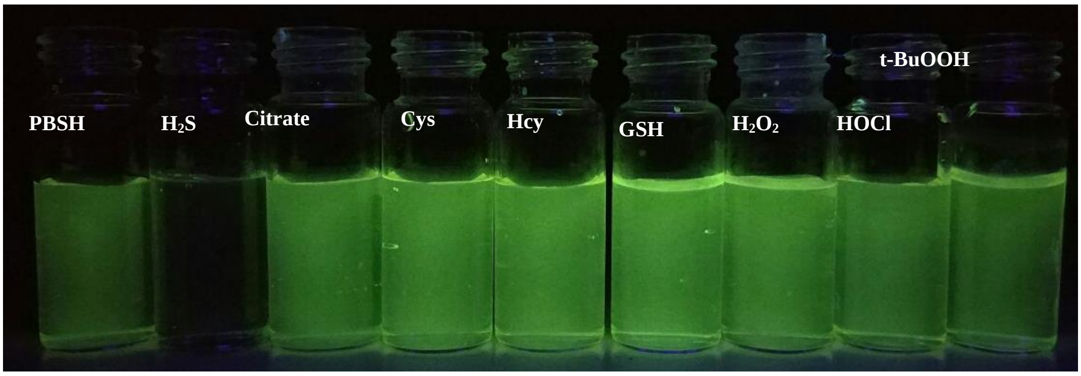
The homeostasis of short-lived reactive species such as H_2S/HOCl in biological systems is essential for maintaining intercellular balance. A typical unpleasant rotten egg smell is the odour characteristic of hydrogen sulfide (H_2S), a compound commonly found in terrestrial and biological ecosystems. An exact redox balance between ROS (Reactive Oxygen Species) and RSS (Reactive Sulphur Species) is essential for the active maintenance of cellular processes such as cell proliferation, differentiation and apoptosis. H_2S is an RSS as well as a reducing agent. Therefore, any imbalance in biological H_2S levels is detrimental to the immunological well-being of organisms. H_2S is known as the third most abundant gas-transmitter following nitrous oxide (NO) and carbon monoxide (CO). Apart from biological applications, there is widespread use of H_2S in industries such as in the production of elemental sulfur and sulfuric acid. Hypochlorous acid (HOCl) is a ROS of notable interest. HOCl fascinates the interest of scientists because of its vital role in pathophysiological processes. Endogenous HOCl is an effective natural oxidant so it can react with proteins, DNA, RNA, fatty acids, and cholesterol and is thought to play vital roles in living systems. There is a growing need to develop molecular probes for the qualitative and quantitative detection of H_2S and HOCl at the macro and microscopic levels. In this lecture some of the recent probes developed by our group for the endogenous and exogenous detection of ROS and RSS will be discussed.





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IL-02

Ionic Liquids: Molecules to Micelles and Gel Materials

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Ionic liquids (ILs) consisting entirely of ions have unique properties and applications. The ionic liquid architecture offers a molecular platform where the ILs can be designed and tailored to consist of various alkyl cations and a variety of anions suiting to the defined and required application. My talk would present our results on the synthesis of amphiphilic ionic liquids based on alkylimidazolium or alkylmethylpiperidinium cations and halide or OH or acetylsalicylate anions in terms of molecular interactions, hydration, surface activity and micellar behavior. The micellar solutions especially of amphiphilic surface active ionic liquids (SAILs) with drug anion are transformed to the gels that can be used as carrier and release systems. The detailed measurements and results would be discussed to correlate the micellar and gelation behavior with the molecular architecture and interactions within the SAILs or SAIL hydrates. The experimental conditions for the formation of micelles and gels are established and would be highlighted. The micellar features were assessed by variety of simple to sophisticated equipment methods tensiometry, steady state fluorescence or quenching, translational diffusion coefficients and small angle neutron scattering. Gelation features were examined in steady state and dynamic oscillatory conditions. The unique molecular interactions between the cation and anion, or SAIL. Water molecules were assessed and adjudged from experimental and density functional theory (DFT) calculations.

Keywords: Ionic liquids, molecular interactions, surface activity, micelles, gels

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IL-03

Fluorescent Chemical Tools for Sub-cellular Imaging

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The desirable chemical, optical, electrical, and biological properties of donor-acceptor (D–A) conjugated organic molecules provide an attractive platform for designing and fabricating newer functional materials. These conjugated materials emitting at lower energy regimes and exhibiting charge transfer are of great interest to diagnostic/analytical applications. Our research interests focus on the design and synthesis of D-π-A molecular systems and investigate their photoresponsive properties for their use in organic electronic or biological applications. Using appropriately substituted auxochromes, we could obtain chromophores with substantial intramolecular charge transfer (ICT) with emission maxima >650 nm and moderate Stokes' shifts. The emission properties were utilized for staining sub-cellular organelles such as plasma membrane, lipid droplets, and mitochondria. In this presentation, our group's recent research findings shall be presented.

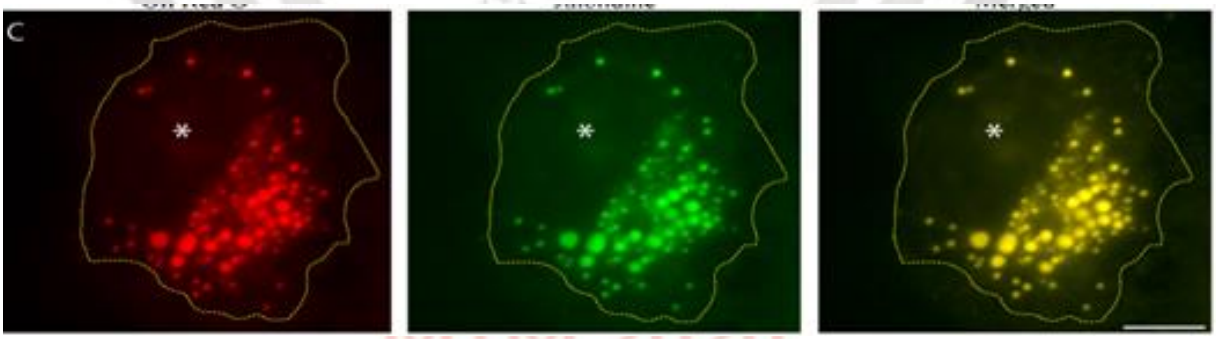

Figure: Imaging of Lipid Droplets using a fluorescent dye

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IL – 04

Potential of Nanomaterials for Chemosensor Development & Water

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The challenge for this century lies in cleaning-up the waste generated during industrial, domestic, and agricultural activities. Water pollution is undoubtedly one of the major problems faced by the world today. Advances in nanoscale science and engineering suggest that many of the current problems involving water quality can be resolved using nanosorbents, nanocatalysts, bioactive nanoparticles, nanostructured catalytic membranes, nanoparticle enhanced filtration, among other products resulting from the development of nanotechnology. Nanomaterials can also be functionalized with various chemical groups to increase their affinity toward some sets of pollutants. They can also serve as high capacity and recyclable ligands for toxic metal ions, radionuclides, organic and inorganic solutes/ anions in aqueous solutions. This presentation will highlight the application of nanomaterials as critical components for purification and to monitor the quality of industrial and public water supply.

IL – 05

Electrochemical Potential Driven Ultra-Thin Films for Molecular Electronic Devices

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Recent advances in the area of molecular electronics reveal that conducting sp^2 carbon electrode can challenge conventional metallic electrode for molecular device fabrication. Functional organic molecules such as aryl diazonium can easily be electrochemically grafted on carbon electrode with desired thickness.[1-3] Carbon-carbon (substrate-molecule) bond is highly thermally stable and thus suitable for low to high temperature range charge-transport studies. In this talk, I would focus on charge-transport properties of conjugated organic molecules of 5-10 nm thick electrochemically grafted on conducting sp^2 carbon electrode followed by carbon top contact fabrication. A strong shielding effect in charge-transport across mobile ions (Li^+) containing bilayer, fluorene-benzoic acid (FL4.5$_{\text{nm}}$-BA4$_{\text{nm}}$Li) probed by regular current density-applied bias (J-V) measurements, fast pulses (50 μs), electrical impedance spectroscopy.[4] The carbon-based molecular junctions hold fascinating potential to replace metal contacts and actually the "tip of the iceberg" for studying electronic and spintronics devices.

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IL – 06

Nature Inspired Smart Self-Healing Materials for Sustainable Disruptive Technology Development

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Exponential demand of smart & sustainable products for different growth sectors are key drivers for disruptive materials and technology development. Self-healing polymers belong to an important class of emerging materials. These materials are focus of attention in both academia and industry due to their diverse commercial potential and beneficial merit for the society at large. A number of innovative approaches have been employed based on molecules such as olefins, di-olefins, sulfur etc. to synthesize materials with capability of self-healing characteristics. The present talk will cover our work in the research area of self-healing materials involving ionic as well as covalent interactions and its applications. The introduction of self-healing property into the polymeric material allowed the repair of micro crack and prevention of crack propagation process. This could be achieved either due to change in temperature or pressure or any other suitable stimulus.

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IL – 07

Hydrogen Bond Interaction in Ionic Liquids: from Fundamental to Application Perspective

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Ionic liquids (ILs) are the type of molten salts, composed of the cations and anions, which are in their liquid phase at relatively low temperatures. The exciting physicochemical properties of ILs originated from the combination of variety of cations and anions, that govern the manifold properties, depict the promising applications in Li+ ion batteries, fuel cells, dye-sensitized solar cells, super capacitors, as well as the utilization of the hazardous gas [1]. Among the various type of interactions in ILs, the hydrogen bond interaction plays a vital role for significant determination of the physicochemical properties of ILs [2]. Therefore, the fundamental understanding of cation-anion interaction and molecular structure properties relation is highly required for the potential use in vast applications. In the present talk, I will discuss the fundamental interaction between the imidazolium based cation and halide anions in ILs in the vicinity of the combined approach of spectroscopic techniques (Raman, IR, and UV-Vis) and density functional theory (DFT) calculations. The effect of size and electronegativity of halide anion on the hydrogen bond interaction in ILs will be discussed [3]. Further, the systematic mixture of water on the ion-pairs will be explored, where how the cation-anion strength and the rotational isomerism of ethyl chain changes under the high dilution of water will be elaborated using the intensity and wavenumbers in Raman spectra and DFT calculations [4]. For the first time using IR spectroscopy, we have investigated the impact of alkyl chain length on the spectroscopic features, which determine the structural and physicochemical properties [5]. As an application perspective, the hybrid structure of ILs and ZnO nanoclusters have been prepared and enhanced the performance for dye-sensitized solar cells. Moreover, we have also investigated the ILs for adsorption of hazardous gases such as (CO_2, SO_2, H_2S and CO). The mechanism of adsorption is discussed using the DFT calculation of adsorption energy, heat of adsorption, vibrational analysis and atoms-in-molecules (AIM) theory.

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IL-08

Pt(II) based anticancer drug design and drug development

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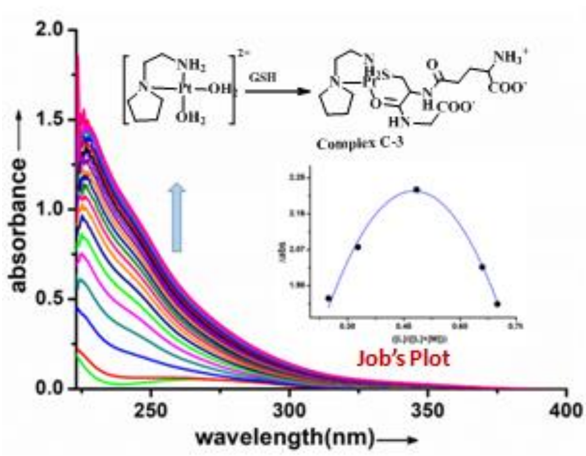
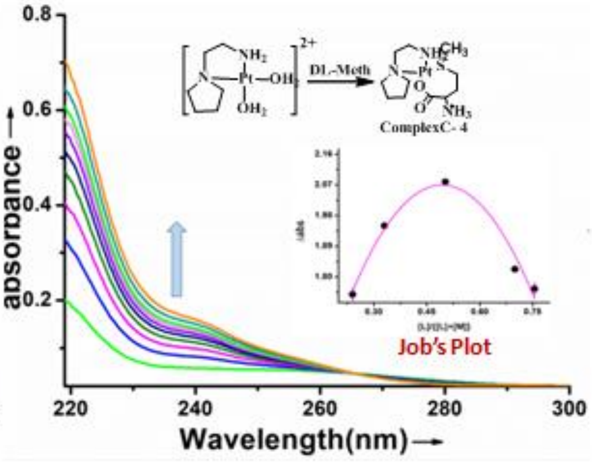
Heterocyclic or aliphatic diamine chelated anticancer agents [1-3] of Pt(II) complexes [Pt(Dim)Cl_2] C-1, [Pt(Diam)(H_2O)$_2$]$^{2+}$ C-2, [Pt(Diam)(GSH)] C-3 and [Pt(Diam)(DL-meth)] C-4 (where, Diam = Diamines) were synthesized and characterized by single crystal/ PXRD and spectroscopic methods. Kinetic investigation with bio-relevant molecules was investigated and their ‘Drug reservoir’ mechanisms are proposed from the calculated activation parameters ($\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$) and rate constants for both steps (k_1 & k_2). Theoretical investigation is also another part of this research work for structural optimization, HOMO-LUMO energy, TD-DFT, NBO analysis and IRC. DNA and BSA binding activity of the complexes were investigated by UV-Vis and fluorescence spectroscopic methods. The mode of binding and binding constants of the complexes with DNA were examined and calculated to compared with other standard Pt(II) diamine complexes for further investigation of their anticancer drug activity. Gel electrophoresis experiments and molecular docking were performed to observe the interaction of the complexes with CT-DNA. In vitro BSA binding activity of the complexes was under consideration as model ‘drug reservoir’ and ‘transport medium’ for carrying Pt(II). A molecular docking with protein and DNA study were explored to evaluate the potential binding mode of the Pt(II) complexes. Anticancer activity of the complexes was studied with Hep-G2, A-549 and normal cell lines and their IC_{50} values were compared with well-known anti-cancer drug cis-platin and other recognized drugs. ROS generation activity on normal cell also measured and compared with ciaplatin, indicates better than traditional drug. Remarkably, all these complexes were tested by NBT assay on normal cell line skeletal muscle cells (L6 myotubes), which revealed that these complexes have minimum adverse effect compared to recognized anticancer medications. The ultimate aim is to explore the cell death mechanism for which cell cycle study has been performed by flow-cytometer with the complexes on HEp-2 cell lines.

Keywords: Anticancer drug; Pt(II) complex; DNA and BSA binding; DFT study and cell death mechanism





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IL– 09

Band Structure Engineering in Two Dimensional Metal Chalcogenide Photocatalyst for Enhanced CO_2 Reduction efficiency under Visible Light

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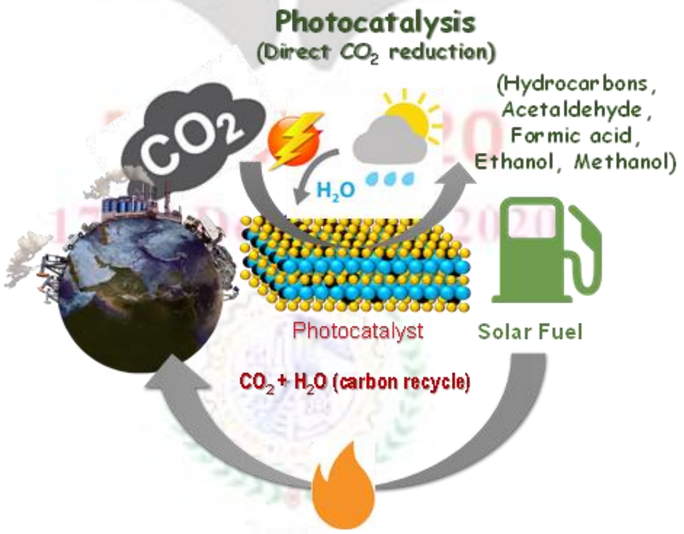
World's geography and climate provide an abundance of solar light and water as free natural resources. We believe that the conversion of CO_2 and water into solar fuels via solar light is an approach capable of tackling both energy and environmental issues and addressing future prospects via efficient, cost-effective solar fuel production. However, efficient implementation of this process, which mimics natural photosynthesis, is technically very challenging, since it involves a combination of processes that can interfere with each other. Last several years, we have introduced several efficient novel nanomaterials (GOs, Cu-GOs, Ni-black TiO_2, C-doped SnS_2 etc.) for this artificial photosynthesis research. To hunting more efficient photocatalyst system recently, bandgap engineering in the metal chalcogenide based photocatalysts represent an important contribution towards high quantum efficiency (nearly 1%) artificial photosynthesis based on gas phase photocatalytic CO_2 reduction under visible light. The details catalyst material synthesis, photocatalytic performance, quantum yield, product selectivity of solar chemicals and recent work will be discussed in the presentation.



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IL – 10

New Thorium (IV) Selective Sensors

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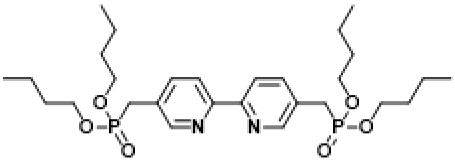
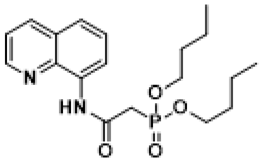
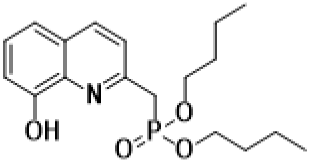
The design and development of chemosensors have expanded substantially in last few decades. In particular, light driven molecular sensors has attracted considerable attention as a type of facile and efficient detection method for sensing chemical species because of their simplicity, versatility, high selectivity and sensitivity. Synthesis of new chemosensors for detection of *f*-metals have been of great interest for chemists. In recent years as they play important roles in the areas of chemical, biological and environmental systems. Based on the above-mentioned evidence, in this presentation, sensing materials such as tetrabutyl ([2,2'-bipyridine]-5,5'-diylbis(methylene))bis(phosphonate) (S_1), dibutyl (2-oxo-2-(quinolin-8-ylamino) ethyl) phosphonate (S_2) and dibutyl (8-hydroxyquinolin-2-yl) methyl phosphonate (S_3) have developed as chromogenic, fluorogenic optode and potentiometric sensor for Th(IV) ions. The lowest detection limit of Th (IV) by S1, S2 and S3 sensors were found to be 2 ppm, 1.1 nM and 1.2 ppm respectively. All three sensors were successfully applied to estimate the Th(IV) in real time samples such as monazite sand and gas mantles samples. The binding mechanism of sensing material with Th(IV) ions was studied by ^{1}H NMR, ESI-mass analysis and theoretical calculations.


S_1


S_2


S_3

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IL – 11

Pyrenyl-appended triazole-linked sugar derivatives for fluorometric detection of Cu^{2+} and Au^{3+} ions in the aqueous medium

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The selective and sensitive detection of metal ions by using fluorescent chemosensors have gained immense interest in recent years for their applications in biology, medicinal and synthetic chemistry. Sugar moiety for the design and development of chemosensors have been used effectively due to several advantages of carbohydrate moiety such as cheap, biocompatible, biodegradable, low toxicity, ring-flipping capability, chiral entities with hydroxyl groups and abundantly available in nature. The triazole group in the sensors provides suitable Au^{3+} or Cu^{2+} binding sites and acts as a linker between the sugar moiety and fluorophore. Sugar-modified pyrenyl-appended triazole-linked sensors have been used for the detection of Au^{3+} and Cu^{2+} ions in water and organic medium. The formation of ligand-metal complexes has been analyzed by UV-vis spectroscopy, fluorescence spectroscopy, mass spectrometry and finally supported by DFT calculations. Additionally, to establish the practical application of the sensors, cell imaging studies were carried out in breast carcinoma cells (MDA-MB-231).

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IL – 12

Chemiluminescent Material and Its Application

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The phenomenon of cold emission of light is known as luminescence. Luminescence process involves at least three steps i.e., energy absorption causing electronic excitation, storage of absorbed energy and emission of photons. Based on type of energy absorbed there are numerous types of luminescence in which chemiluminescence (CL) and bioluminescence (BL) are natural phenomena that have attracted the attention of mankind since the evolution of life on the earth. Chemiluminescence, the production of light during a chemical reaction, has proved to be a useful phenomenon in the laboratory and is finding ever increasing applications in analytical chemistry. Explorations of CL for analytical applications have been continual since the 1970s and 1980s for the gas-phase and liquid-phase reactions, respectively. Analytical applications of chemiluminescent material are well reported in various disciplines including biomedical, food, environmental and toxicological analysis. In present paper, the employability of chemiluminescence are highlighted in the estimation of different environmental samples for continuous monitoring. The characterization of tropospheric O_3, NO_X, $NH_3$and other atmospheric pollutants with the context of recent technological developments arewell discussed.

IL – 13

DNA based, monofunctionalized quantum dots for single particle bioimaging of proteins in living cells

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Functionalization of quantum dots (QDs) with a single biomolecular tag using traditional approaches in bulk solution has met with limited success. DNA polyhedra consist of an internal void bounded by a well-defined three-dimensional structured surface. The void can house cargo and the surface can be functionalized with stoichiometric and spatial precision. I will present a new method of producing monofunctionalized QDs can be realized by encapsulating QDs inside DNA icosahedra and functionalizing the DNA shell with an endocytic ligand. I will present how DNA-encapsulated QDs can be explored for real-time imaging of three different endocytic ligands-folic acid, galectin-3 (Gal3) and the Shiga toxin B-subunit (STxB). Single-particle tracking of Gal3- or STxB-functionalized QD-loaded DNA icosahedra allows us to monitor compartmental dynamics along endocytic pathways. Using lattice light sheet microscopy, we were for the first time able to quantify the whole cell endocytic events and classify them systematically into various endocytic uptake routes in cells. These DNA-encapsulated QDs, which bear a unique stoichiometry of endocytic ligands, represent a new class of molecular probes for quantitative imaging of endocytic receptor dynamics.

Keywords: Structural DNA nanotechnology, 3D cages, Monofunctionalized quantum dots, Single particle tracking, Lattice light sheet microscopy

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IL – 14

Application of graphene nanosheets in drug delivery: possibilities and challenges

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Graphene, a one-atom thick nanocarbon, displays a unique honeycomb structure and extensive conjugation. It exists in various dimensionality; from few micrometer sheets (with irregular surface) to ultra-small quantum dots. Methods are evolving to produce defect-free and stable sheet dispersions. Apart from high surface area-to-mass ratio, graphene displays unique optical, thermal, electronic and mechanical properties. Its optothermal properties are appealing from the standpoint of multimodal drug delivery, imaging and biosensing applications. The hydrophobic basal plane can be efficiently loaded with aromatic drug molecules via non-specific forces. In spite of these interesting properties, biosafety of graphene remains questionable due to its non-specific binding affinity for drugs, protein, nucleotides and cellular components. Besides, it quickly aggregates in physiological solutions and the resulting polydispersity vandalizes the size-dependent properties.

The toxicity of sheets depends upon their interaction with blood components, physical adsorption over cell surface and trans-cellular migration to manipulate cytosolic processes. Our studies suggest that events related to sheet aggregation can be minimized through surface functionalization. The technique affords new biological identity and overall hydrophilicity to the sheet surface. Nevertheless, the success of this approach strategy leans over comprehensive understanding of surface chemistry, surface forces and energetics of graphene-stabilizer interaction. This research talk is aimed to discuss our approach of imparting superior aqueous dispersity to the sheets using block copolymer micelles.

IL – 15

Green and sustainable developments for various value added organic transformations

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There is a strong need to develop the green, economical and highly efficient catalytic methods in organic chemistry, pharmaceutical chemistry and fine chemical industries. Present scenario demands to revive the R&D of the existing traditional organic methods those are used for the large scale synthesis of various chemicals. The synthesis of various basic and value added products which includes biphenyls, acetones, amides, aldehyde, acetal, thiol, dithiane and amine derivatives etc. are not only multistep but also demand the presence of Nobel and expensive metals (Pd, Rh, Ir and Ru), toxic solvents and rigid reaction conditions. The present lecture will be focused on the developments of various new green methodologies which are highly economical, strongly feasible and sustainable for environment.[1-2] The catalytic activity of 3d abundant metals is still challenging due to the low catalytic potential, hence, some latest green catalytic developments based on 3d metals will be shared during the presentations.[3-5]

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IL – 16

Catalytic Converters for Control of Pollution from Automobile Exhausts

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This talk will brief on an overview of various emission control technologies employed to meet stringent vehicular emission standards worldwide. The vehicular emission exhaust gases consist of CO, hydrocarbons, NOx and particulate matters. The most common technologies used to convert the emission exhaust gases into environmentally benign gases are three-way catalyst, diesel oxidation catalyst, diesel particulate filter and selective catalytic reduction, depending on the fuel and engine technology issued in the internal combustion engines.

The industry for manufacture of emission control systems from automobile exhaust has evolved as a niche high technology area that is the largest market for precious group metals, platinum, palladium and rhodium. The key to efficient and optimal use of the precious metals is the formulation of the catalyst carriers and its application as a washcoat on metallic and ceramic substrates. This talk attempts to describe the development as well as the challenges that lie ahead in meeting the ever increasing stringency of the norms for tail pipe emissions from automobiles.

IL – 17

Iron Oxide Nanosheets and their potential applications

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Nanoscale will have far reaching impact and the next revolution in science and technology will depend on science interdependence. The future of nanotechnology is likely to continue in interdisciplinary manner. Physical, chemical and biological will merge with an understanding that tools and principles at lower scale are same.

Bio-safe and bio-compatible route have been explored. The present work reports the formation of sheets like morphology of iron oxide via the anodization of Fe sheet in ethylene glycol (EG) electrolyte. XRD, FESEM, EDX, DRS, and Raman are applied to characterize the samples. SEM results verified the sheets like morphology. The average width of the nanoflower petal is ~25 nm and the length are about 80nm. XRD and Raman results indicate that all the fabricated nanostructures consist of magnetite, which transforms into hematite by annealing. The formation of nanosheets-like morphology can be attributed to EG. A possible formation mechanism of nanosheets is proposed. We showed that the morphology of the as-anodized iron oxide can be tailored simply by changing the electrolyte. Moreover, photocurrent density of as such fabricated iron oxide nanoflowers were studied using electrochemical analyser and found that the photocurrent density is of 0.7 mA cm^{-2} which reveals their potential in harvesting light energy in visible region of solar spectrum significantly. In addition, the method is economical, environmentally benign, involves green chemistry, which can make it suitable for scale large production. The prospects of the process are bright and promising. There are number of applications which shall be discussed during the talk.

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IL – 18

Theoretical Calculations on Materials: Computational Approach

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Computational calculations using Density Functional Theory (DFT) provides a deeper understanding of structure and bonding in the materials. Periodically extended systems are conveniently modeled in DFT using plane-wave basis set approach. The present talk will be focused on delivering the DFT based computational approaches for fundamental calculations on materials such as geometry optimization of materials, single-point energy calculations, calculations of optical properties like phonon dispersion relation, density of energy states and phonon vibronic states, calculations of dielectric constant, band-gap, etc. of materials, etc. A general idea about DFT will be discussed during the talk to familiarize the audience with the field. Some examples will also be discussed to illustrate the applications of DFT to calculate some of mentioned material properties for certain simple systems. Further, as it is well known that DFT underestimates the band-gap of materials, incorporation of essential corrections will also be discussed to account for these limitations of the method.

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IL-19

Biopolymer Adsorbents with Tunable Uptake Properties for Anion Species

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The uncontrolled release of nutrients in aquatic environments globally and the resulting effects of eutrophication and excessive algae growth have created a need for sustainable water treatment methods. Biopolymer materials have promising potential as adsorbents for the controlled removal of oxyanion species in water and wastewater due to their molecular tunability and sustainability. This presentation will provide an overview of research progress at the University of Saskatchewan related to the design and characterization of biopolymer platforms as adsorbent materials for uptake of environmentally relevant anions. In particular, case studies of sorbents with high affinity toward oxyanion species are described, where synthetic modification of biopolymers in a modular fashion (surface functionalization, cross-linking, and composite formation) reveal enhanced physicochemical properties related to adsorption and responsive behaviour to external stimuli [1,2]. Selected examples of molecular materials that show reversible adsorption–desorption processes and high efficiency of oxyanion removal are highlighted. This research contributes to the development of advanced biosorbent materials for controlled removal of oxyanion waterborne species for sustainable water treatment processes [3-5].

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IL-20

Synthesis of heterocyclic molecules under catalyst-free, homogeneous and heterogeneous catalysis conditions in aqueous medium

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Synthesis of heterocyclic compounds is one of the fast growing area of synthetic organic chemistry because of many of the commercially sold drugs contain hetero atoms in their structure. Many methods like the use of multicomponent, tandem (cascade) reactions in presence of homogeneous and heterogeneous catalysts and catalyst-free conditions have been developed over the years. Along with above, the development of synthetic methods under green conditions is also one of the aspect of current developments. Considering this, present lecture covers the work (shown in the image) reported from our laboratory from past couple of years using Bi_2WO_6, $BiPO_4$, and ZnO nanoparticles as heterogeneous catalysts in water as reaction medium.

Catalyst-free reactions
- Vinylogous Henry and 1,6-Michael addition reactions
- Domino sulfa Michael / intramolecular Aldol reactions
- Synthesis *bis*-indolyloxindoles via retro-Henry reaction

On-Water and In-Water Organic Synthesis

Homogeneous Catalysis
- Bibenzo-[1,4]-diazepin-1-ones
- Chromenes and spirochromenes

Heterogeneous Catalysis
- Multicomponent reactions
- Sp^3 C-H activation

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IL – 21

Detailed Mechanistic Investigation of Oxidative 1, 2-Aryl C-C Migration using [Hydroxy(tosyloxy)iodo] benzene in Dichloromethane: In Search of Novel Precursors

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The present study investigates and validates [hydroxy(tosyloxy)iodo]benzene (HTIB) mediated stereoselective and oxidative 1,2-aryl C-C migration in variegated α,β-unsaturated diaryl ketones. This oxidative-skeletal rearrangement ultimately outgrowth to optically active α-aryl-β,β-ditosyloxy ketones in presence of CH_2Cl_2 as non-nucleophilic solvent. The generality of fascinating 1,2-aryl C-C migration was thoroughly investigated and verified by electronic (EDG/EWG) and steric factors on different derivatives of α,β-unsaturated diaryl ketones. Mechanism of 1,2-aryl C-C migration has been very well studied with the help of Density Functional Theory (DFT). Aesthetically this novel and unique three carbon component would expose a direct and conceptually robust strategy to access regioselective synthesis of 4,5-diaryl isoxazole, 4,5-diaryl pyrazoles and 1,4,5-triaryl pyrazoles and also efficient access to desoxybenzoin and other important β,β-difunctionalized chemical entities.

Keywords: Oxidative Rearrangement, β,β-Bifunctionalization, α-Aryl-β,β-ditosyloxy ketones, Hirshfeld surface, Frontier Molecular Orbitals (FMOs), Electrostatic Potential.

IL – 22

Hydrothermal conversion of household food waste to hydrogen-rich syngas production

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Significant amounts of fruit wastes and agro-food residues are generated worldwide as a result of food processing. Fruit residues contain numerous bioactive components, such as carbohydrates, lipids, fats, cellulose, hemicellulose and lignin that have tremendous potentials to be converted into biofuels. Food wastes are usually disposed of in landfills or incinerated raising several environmental concerns and health risks. This study highlights the characterization and hydrothermal gasification of several fruit wastes and agro-food residues such as aloe vera rind, banana peel, coconut shell, lemon peel, orange peel, pineapple peel and sugarcane bagasse. The fruit wastes and agro-food wastes were gasified in supercritical water to study the impacts of temperature (400-600°C), feed concentration (1:5 and 1:10 biomass-to-water ratio) and reaction time (15-45 min) at a pressure range of 23-25 MPa. The catalytic effects of NaOH and K_2CO_3 were also investigated to maximize the hydrogen yields and selectivity. The elevated temperature (600°C), longer reaction time (45 min) and lower feed concentration (1:10 biomass-to-water ratio) were optimal for higher hydrogen (0.91 mmol/g) and total gas yields (5.5 mmol/g) from orange peel. However, coconut shell with 2 wt% K_2CO_3 at 600°C and 1:10 biomass-to-water ratio for 45 min of gasification revealed superior hydrogen yield (4.8 mmol/g), hydrogen selectivity (46 %) and total gas yields (15 mmol/g) with an enhanced lower heating value of gas products (1595 kJ/Nm^3). The overall findings imply that supercritical water gasification of fruit wastes and agro-food residues could serve as an effective organic waste management technology with regards to bioenergy production.

Keywords: Food Waste; Supercritical water gasification; Hydrogen; Synthesis gas; Alkali Catalysts; Biochar.

IL-23

Nanoadsorbents: the efficient materials for decontamination of metal rich wastewaters

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Water pollution has always attracted scientific workers as global availability of fresh water was never adequate. Solution to this problem seems to come from treatment of wastewater and its reuse. Wastewater treatment and water purification have always posed challenges to mankind and this problem has become severe with escalating population and industrialization. This topic has attracted the global scientific community. Activated carbon adsorption became popular choice for water purification but its high cost prompted scientific workers to search for its alternates. In that series, several materials including minerals, waste materials, cellulosic materials, etc. were also applied as adsorbents. After advent of nano technology, there was a shift towards application of nano materials as 'adsorbents' and the term was coined as 'nano adsorbents' by our group. This lecture focusses on application of several nanoadsorbents synthesized in our laboratory and then applied for decontamination of metal rich water and wastewaters.

Keywords: Metallic species; Nanoparticles; Removal; Wastewater.

LINKS FOR PRESENTATIONS:

Google meet Link-1
(Inauguration, Keynote lectures and Parallel session-1)
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Google meet Link-3
(Parallel session-3)
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Topic: Special Talk by Nobel laureate Prof. Jean-Marie Lehn
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YSA-01

A unique strategy to obtain bright-white-light emission via controlled energy transfer from a ligand to Eu(III) ion: its versatile applications

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The new single-organic-molecule or molecular-complex based white-light-emitting sources are attractive owing to their potential applications in full-color smart displays and lighting sources. In general, white light can be generated by mixing three primary colors, to cover the entire visible spectrum. At present, several organic fluorophores having the capacity of emitting individual red-blue-green (RGB) color are known. However, white light generated by a single molecule (a single-component approach) has several advantages over that of simple RGB mixing (multicomponent emitters). The benefits include improved stability, stable Commission International de I'Eclairage (CIE) color coordinates, and a simple fabrication process.

In the part of above contemporary, a new diphenylamine-functionalized ancillary-ligand-coordinated Europium (III) β-diketonate complex is designed ($Eu(TTA)_3$Phen-Fl-TPA-DPA) and synthesized. It has showed incomplete photoexcitation energy transfer from a ligand to a Eu^{III} ion. A solvatochromism study led to a balancing of the primary colors to obtain single molecule white-light emission. The photophysical and electrochemical analysis were carried out experimentally as well as theoretically (DFT, TD-DFT) and shown appropriate CIE color coordinates. Eu-complex intensive characteristic red emission at 612 nm is due to the intra-configurational $^5D_0$ -^7F_J (J = 0 - 4) electronic transitions. Thermal-sensing analysis of the europium complex was executed. The europium complex, conjugated with a near-UV-light-emitting diode (395 nm), showed appropriate white-light-emission CIE color coordinates (x = 0.34 and y = 0.33) with a 5152 K correlated color temperature. The detailed investigation to be presented and discussed.

Keywords: Europium, antenna, LED/ OLEDs, Temperature Sensor.

YSA-02

Polymorphs, Co-crystals, Protein Binding and Cytotoxicity of Some Quinone Derivatives

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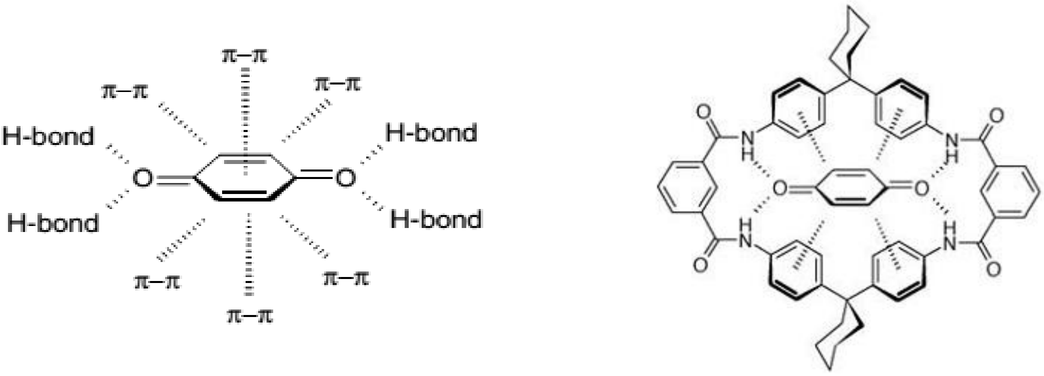
Quinones and derivatives form self-assemblies guided by various weak interactions such as O-H···O, C-H···O, C-H···π and O-H···π interactions. Presence of strong directional hydrogen bonds in quinoidal compounds form hydrogen bonded assemblies which may be in the form of linear or cyclic assemblies. There are several characteristic supramolecular features associated with substituted quinones.[1] Polymorphism is a phenomenon of a substance having several different crystal forms or modifications. Whereas co-crystal is a crystalline structure made up of two or more components in a definite stoichiometric ratio, where each component is defined as either an atom, ion, or molecule. Polymorphism has received immense practical importance in pharmaceuticals as each polymorph can exhibit different chemical and physical properties including dissolution rate, bioavailability, stability, melting point, solubility, optical and mechanical properties, vapor pressure, etc.[2a] When different conformers of a molecule occur in different crystal forms, phenomenon is termed as conformational polymorphism.[2b] Polymorph stability is of special interest because their energy differences are relatively small and inter-conversion is very common. Conformational energy change or rotation about single bonds (torsion) of a molecule is within range 1-3 kcal mol^{-1} or it can go up to 7-8 kcal mol^{-1}; that may lead to conformational polymorphs. Energies of intramolecular torsions and intermolecular non-bonded interactions lie in the same range (0.5-10 kcal mol^{-1}).[1-2] So, a conformationally flexible system with provision of weak interactions would show polymorphism. Polymoprhs are formed as a consequence of difference in crystal structures. They also show different vibrational spectra and diffraction patterns are shown in figure 1a.



(a) (b)

Figure 1: (a) Sites for supramolecular interactions in the *p*-benzoquinone and (b) *p*-benzoquinone as a guest in a host-guest complex.

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YSA-03

Parabens induced spherical micelle to polymersome transition in thermo-responsive amphiphilic EO-PO block copolymers

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Micellar transition induced employing pharmaceutically-active antioxidants specifically *p*-hydroxy benzoic acid esters (parabens) *viz.*, methyl paraben (MP), ethyl paraben (EP), propyl paraben (PP), butyl paraben (BP), benzyl paraben (BzP) in ~ 5 %w/v thermoresponsive triblock *linear*: Pluronic® (P84) and *star-shaped*: Tetronic® (T1304) copolymers was investigated in aqueous solution. The solution behavior of these block copolymers in presence of parabens is well scrutinized from cloud point (CP), relative viscosity (η_{rel}), spectral (FT-IR, UV-vis), computational simulation, and scattering (dynamic light scattering (DLS) and small angle neutron scattering (SANS)) study. Varied phase behavior and a dramatic change in η_{rel} with temperature ageing is attributed to the plausible induced micellar transition (spherical micelle to polymersomes) which is accounted to the involved hydrophobic interactions therein as depicted from spectral study and further rationalized using computational simulation approach. The prominent shifts observed in the hydrodynamic diameter (D_h) of parabens loaded and unloaded copolymeric micelles was inferred from DLS while SANS findings clearly depicted the micellar dimensions with the aggregation number (N_{agg}). Furthermore, the performed antioxidant (*free radical scavenging* and *reducing capacity*) assay in non-micellar and micellar media trait the ability to shuttle between the reduced and oxidized forms that prevents the oxidative damage which is biologically important.

Keywords: EO-PO block copolymers; parabens; phase behavior; micellar transition; scattering; antioxidant assay.

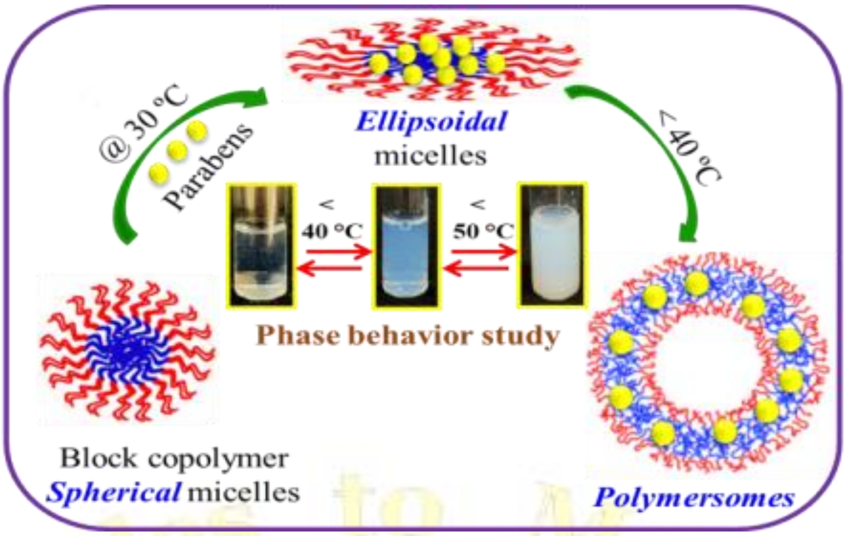

Figure: Parabens loaded in block copolymeric micelles thereby inducing micellar transition with temperature ageing.

YSA-04

Group-V bilayers for promising visible-light photocatalysts application with higher carrier mobility

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We have systematically studied the structural, electronic, transport and photocatalytic properties of SiX (X = N, P, As, Sb, Bi) homo-bilayers considering five different possible stacking configurations. The dynamical stabilities of all the systems are tested by calculating their phonon dispersion spectrum, suggesting that odd stackings are dynamical stable. The electronic band structure study reveals that SiX homo-bilayers are moderate band gap semiconductors with an electronic band gap of 2.488 eV – 0.948 eV calculated using HSE06 functional. Using the deformation potential theory and effective mass approximation, the electronic transport properties reveals ultrahigh carrier mobilities of the order of 10^6 cm^{2}V^{-1}sec^{-1}. Interestingly, we observed that the band edge potentials of SiP and SiAs qualifies the oxidation and reduction potentials for overall photocatalytic water splitting. Further, optical absorption studies shows absorption in the visible region for SiN, SiP, and SiAs indicating its potential for photocatalytic water splitting. This indicates the potential of SiP and SiAs homo-bilayers to be used as visible light photocatalytic water splitting application.

Keywords: Group IV-V binary compounds, deformation potential theory, carrier mobility, photocatalytic water splitting, optical absorption.

YSA-05

Study of Anticancer Drugs Interaction with Hemoglobin by Electrochemical Spectroscopy and Molecular Docking: Implications towards Anticancer Treatment

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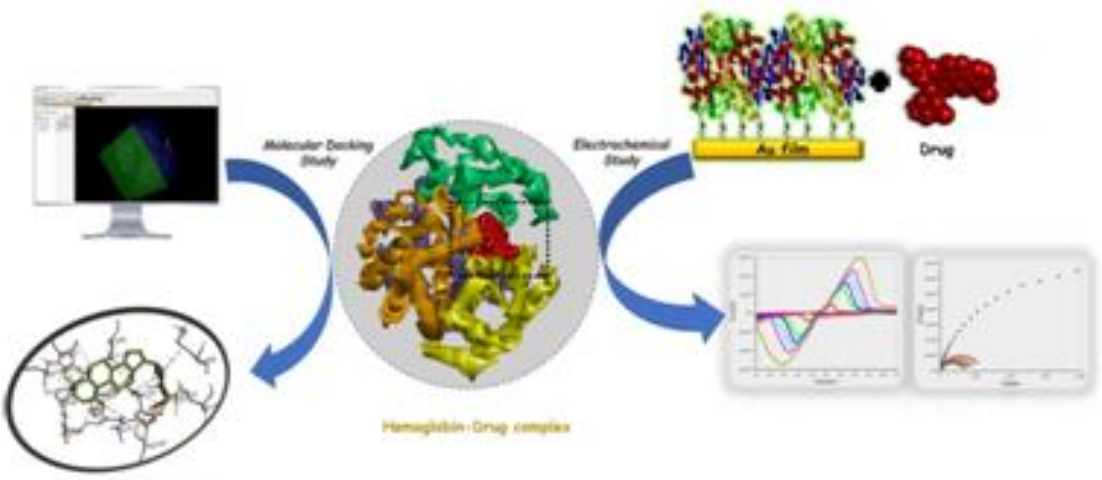
Hemolysis is a major side effect while chemotherapy. Here we studied the Interaction of chemotherapeutic drugs with Hemoglobin by electrochemical method and molecular docking. The immobilization of Hemoglobin on the Au surface facilitates the study of direct interaction between Hemoglobin and anticancer drugs. Electrochemically active drugs are selected for this purpose i.e., Doxorubicin and 5-Fluorouracil. Doxorubicin undergoes a reversible two-electron reaction and charge transfer resistance decreases with an increase in the concentration of doxorubicin while interacting with Hemoglobin. In contrast, 5-Fluorouracil shows only oxidation reaction, and variation in charge transfer resistance is not that significant. The molecular docking complies with electrochemical study, depicting binding sites of drugs at the Hemoglobin surface. Thus, this enriches our understanding of electron transfer reaction between chemo drugs and hemoglobin, which will help to design new chemotherapy methods with fewer side effects.



YSA-06

TTAB and natural template mediated synthesis of mesozeolite H-BEA, characterization and its application in the synthesis of valuable butyl ester

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Zeolites are microporous anhydrous crystalline aluminosilicate materials having very well-defined and regular pore structures of molecular dimensions. They are most promising candidates for wide range of applications in the area of catalysis, water softening, separation, storage etc., because of their high surface area, high instrinsic acidity, thermal stability and shape selective property [1]. However, the microporous zeolites are suffering from diffusional limitations when used in organic transformation involving bulkier entities due to its microporous nature of complex pore system, channels and cavities. Hierarchical zeolites belong to one type of advance materials which combines advantages of both microporous (i.e. high acidity and thermal stability) and mesoporous (high surface area and pore volume) while avoiding disadvantages of each. Use of desilication method with surface directing agents [tetradecyltrimethyl ammonium bromide (TTAB) and rice husk] is one of the effective post synthetic route to fabricate hierarchical catalytic materials [2]. In the present endeavour, a meso H-BEA has been synthesized using TTAB and rice husk (biomass waste material), which is less reported research as per authors' knowledge. The resultant mesozeolite material (MTRK) is characterized by elemental, spectral, thermal and surface area analysis. Further, the catalytic activity of MTRK has been assessed towards the synthesis of n-butyl levulinate from levulinic acid (LA) and n-butanol via esterification reaction. In order to evaluate the catalytic activity of MTRK, Box-Behnken Design (BBD) was used to find optimized reaction parameters for obtaining maximum % conversion of LA. In conclusion, MTRK catalyst showed high % conversion of LA into n-butyl levulinate as compared to parent H-BEA. Thus, it can be said that the newly synthesized micro-meso composite MTRK can be a promising material to execute other organic transformations to yield other value added scaffolds and complex biomolecules.

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YSA-07

Study on inclusion complexation between β-cyclodextrin and vitamin B6 cofactor over nanomaterials and their potential applications in sensing

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Inclusion complexation study is always fascinating for exploring interaction between two molecules. Host guest interaction between β-cyclodextrins and other natural and synthetic molecules have been studied by different scientific research and various kinds of interaction have been explored. Most of the research significantly concludes that inclusion complexation greatly affects the physical chemical properties of the guest molecules, such as solubility, chemical reactivity and the spectroscopic, electrochemical properties and their sensing and biosensing ability as well. In this work [1], we studied the host-guest interaction between β-cyclodextrin and vitamin B6 cofactor Pyridoxal 5' phosphate. In our approached, silver nanoparticles and copper nanoclusters by using β-cyclodextrin as a capping agent were prepared and then the inclusion of vitamin B6 cofactor was studied. The nano-assembly developed after the inclusion of vitamin B6 cofactor over the nanoparticles/nanoclusters was applied for the fluorescent turn-on sensing of hydrazine and Al^{3+}.

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YSA-08

Simultaneous determination of five bioactive constituents in fruit rind extracts of Garcinialanceifolia using a validated UHPLC-PDA method and evaluation of antioxidant capacity

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Xanthones and polyisoprenylated benzophenones found in *Garcinia* species are groups of secondary metabolites with a wide range of bioactivities. Three xanthones namely α-mangostin, β-mangostin, γ-mangostin and two polyisoprenylated benzophenones namely xanthochymol and isoxanthochymol were identified and quantified in the extracts prepared from fruit rinds of *G. lanceifolia* using a validated UHPLC-PDA method. Total phenolic content of *G. lanceifolia* extracts of varying polarity was determined by the Folin-Ciocalteu method. These extracts were also evaluated for their antioxidant potential using three different *in vitro* assays namely DPPH free radical, ABTS cation radical and reducing power. α-mangostin was not quantified in hexane and chloroform extracts. β-mangostin could not get quantified in hexane extract. γ-mangostin was not detected in any of the six extracts. Xanthochymol content was the highest (289.26 ± 0.31 mg/g) in hexane extract. Isoxanthochymol content (9.91 ± 0.01 mg/g) was maximum in hexane extract and it was followed by chloroform (2.67 ± 0.01 mg/g) extract. The highest total phenolic content was recorded for hexane extract (18.60 ± 1.95 mg/g GAE). *In vitro* assays established that*G. Lanceifolia* extracts have significant antioxidant activity.

Keywords: Xanthones, polyisoprenylated benzophenones, total phenolic content, and antioxidant activity

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YSA-09

Characterization of molecules structure of polysorbates influenced by sodium salts

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Micellar properties and structural characterization of polysorbates (commonly known as Tween 20 and Tween 80) were investigated in presence of monovalent salts (NaX, X = Cl^-, Br^-, $NO3^-$ *and salicylate*) at different temperatures (30˚C - 50˚C) by using cloud point, densitometry and viscometry methods. These polysorbates belong to the nonionic kind of surfactant. These studies reveal the drastic influence of added salts and temperature on the molecular structure of polysorbates and provide valuable information. Density and viscosity measurements confirmed the molecular structure change. Polysorbates are widely used as emulsifiers in the food industry.

Keywords: Polysorbates, micellar systems, cloud point.

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OP-01

Sensitive and Regenerable Organochalcogen Probes for the Colorimetric Detection of Thiols

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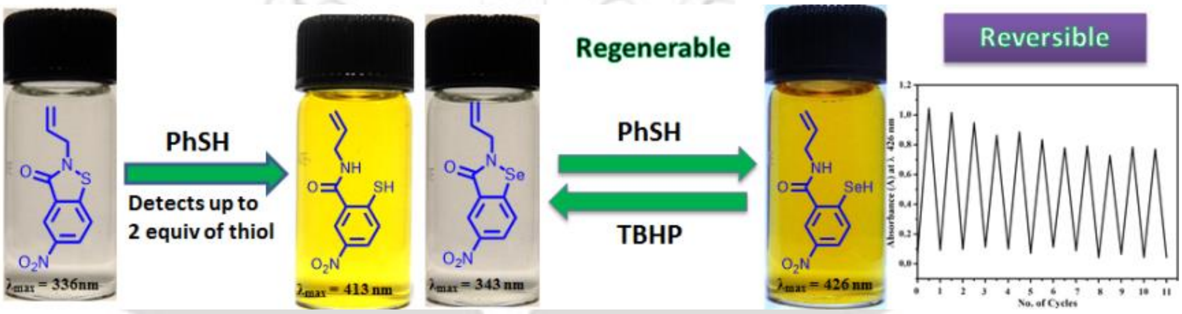
Isothiazolone and Isoselenazolone based probes have been reported for the colorimetric detection of thiols. Isothiazolone probe detects two equiv. of thiols whereas Isoselenazolone based probe detects thiol in a reversible manner for more than 10 cycles. Detailed mechanistic investigation has been carried out for both the probes. Both probes possess higher selectivity for aromatic thiols, cysteine and glutathione. This is the first report of a reversible colorimetric probe for the detection of thiols.



Keywords: Thiol Sensing, Isothiazolone, Isoselenazolone

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OP-02

A simple diaminomaleonitrile based molecular probe for selective detection of Cu(II) and Zn(II) ions in semi-aqueous medium

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A Schiff base probe (**ANTI-DMN**) was synthesized from diaminomaleonitrile and 4-antipyrine carboxaldehyde and found to exhibits high sensitivity and selectivity towards Cu^{2+} and Zn^{2+} in semi-aqueous medium (CH_3CN: H_2O, 7:3 v/v). Upon interaction with Cu^{2+}/Zn^{2+} **ANTI-DMN** showed an instant colour change from colorless to yellow. The sensing ability was further confirmed with various spectroscopic techniques such as UV-Vis, NMR, FT-IR, and ESI-MS. The binding nature of the probe was determined by Job's plot, from this stoichiometric binding ratio of the probe was calculated as 1:1 for Cu^{2+} and Zn^{2+} ions. The limit of detection of Cu^{2+} and Zn^{2+} ions were found to be 0.204 µM and 2.014 µM respectively, which is lesser than the permitted level of WHO in drinking water. The **ANTI-DMN** coated test kit was developed using silica-supported TLC plates, which also observed to display a quick colorimetric response of Cu^{2+} and Zn^{2+} ions. Moreover, the theoretical calculations were performed using the DFT/TD-DFT method. **ANTI-DMN** proved to be an excellent probe for the rapid colorimetric detection of Cu^{2+} and Zn^{2+} ions in a semi-aqueous medium.

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OP-03

Inducing *T1–T2* Dual Contrast Imaging Ability to Iron Oxide Nanoparticles for Magnetic Resonance Imaging: *Surface Environment Matters*

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Ethylene diamine tetra acetate (EDTA) capped Fe_3O_4 nanoparticles (NPs) have been synthesized and encapsulated using polymeric micelles (Pluronic F-127). The synthesized Fe3O4/EDTA/P magnetic micelles are used as a vehicle to load the hydrophobic drug imatinib and transfect it in a bone marrow cell-line (K562) in vitro for the treatment of chronic myeloid leukemia. A phantom study was carried out to determine the relationship between T1 and T2 relaxation times with various concentrations of Fe_3O_4/EDTA/P NPs. In vivo magnetic resonance (MR) imaging conducted on nude mice bearing the synthesized magnetic micelle after i.v. administration reveals excellent imaging capabilities, in dual mode, especially 24 h post-injection. It was observed that the synthesized magnetic micelles act as a *T1–T2* dual contrast agent. We propose that the longitudinal relaxation (T1) of water protons can be induced by mimicking Gd-DTPA chelate chemistry while transverse relaxation (T2) can be achieved by controlling the particle size.

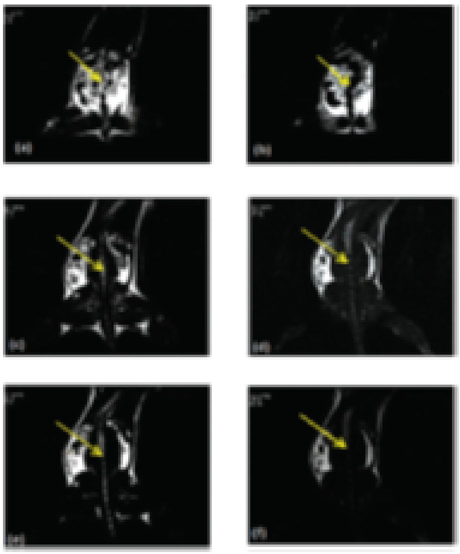

Figure 1.
MR images of synthesized Fe_3O_4/EDTA/P NPs injected into rats: (a and b) T1-weighted and T2-weighted images prior to the injection of NPs, (c and d) T1-weighted and T2-weighted images 15 min post injection of NPs, (e and f) T1-weighted and T2-weighted images 24 h post injection of NPs. Arrows indicate the bone marrow.

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OP-04

Highly Selective Coumarin Hydrozone as Fluorescent chemosensor for Lu^{3+} Determination and Bio-Imaging in Zebrafish

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A new Lu^{3+} selective fluorescent probe **S** was synthesized and characterized. The optical properties of **S** were investigated by using absorption and fluorescence spectral studies in 7:3 (v/v) aqueous dimethyl sulphoxide. Upon addition of Lu^{3+} at pH 4 (acetate buffer) solution of **S**, the weakly fluorescent probe **S** becomes highly fluorescent. The fluorescence intensity was increased five-fold at 490 nm when excited at 437 nm. The formation of 2:1 complexation between **S** and Lu^{3+} was confirmed by Job's plot. The binding constant ($\mathbf{K_a}$= 1.43 $\times 10^4$ M^{-1}) was determined by the Benesi-Hildebrand (**BH**) method. The limit of detection (**LOD**) of Lu^{3+} using **S** was found to be 23 nM. The binding mechanism of **S** with Lu^{3+} was studied by ^{1}H-NMR, ESI mass, and theoretical studies. Further, probe **S** has been successfully used to bioimaging Lu^{3+} in Zebrafish gill cell line (*Dr*G) and zebrafish (*Danio rerio*) in the yolk, papillae of eyes, and head of Zebrafish embryos, therefore providing a powerful live imaging approach for investigating chemical signaling in complex multi-cellular systems.

Keywords: Fluorescent probe, Lu^{3+}, CHEF, Bio-Imaging, Zebrafish.

OP-05

Selective Detection of Fluoride and Hydrogen sulfate Anions by Pyrimidine-based Fluorescence Chemosensor

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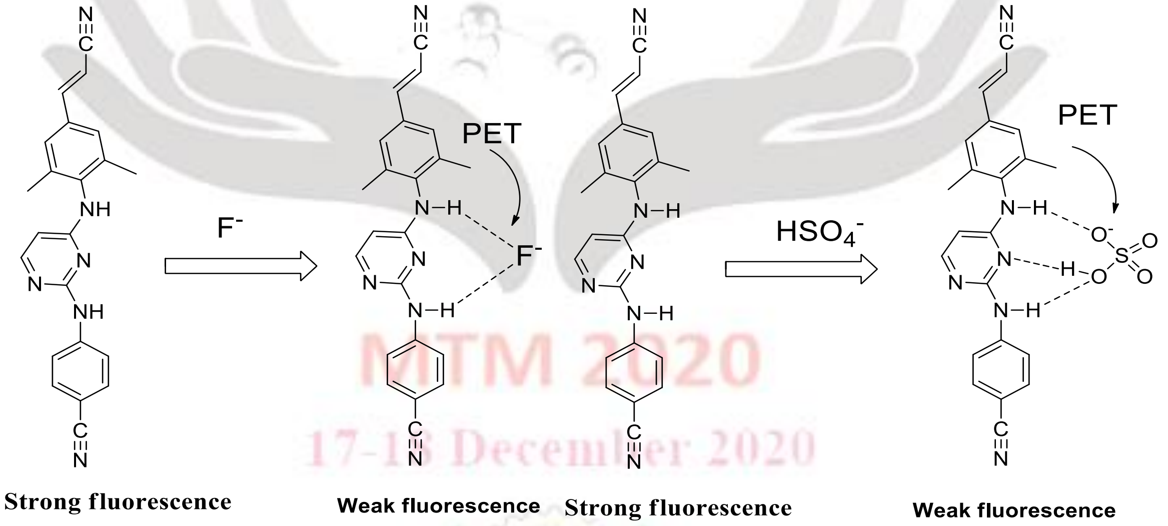
The binding and sensing abilities of pyrimidine based fluorescence chemosensor **L** towards different anions such as F^-, Cl^-, Br^-, I^-, NO_3^-, ClO_4^-, $H_2PO_4^-$ and HSO_4^- was examined by fluorescence spectroscopy in DMSO-H_2O (7: 3, v/v). Upon successive addition of various anions to **L**; quenched the fluorescence emission was occurred at 480 nm. Analysis of fluorescence emission changes recommended that **L** formed 1: 1 complex with anions. From the fluorescence binding constant data, it found that **L** form strong complexes with F^- and HSO_4^-ions through H-bonding interactions. The selective response of F^-over other halides and HSO_4^-amongst other oxo-anions towards **L** may be explained on the basis of photo-induced electron transfer (PET) process.



Scheme 1: Plausible mechanism of (a) **L** with F^-; (b) **L** with HSO_4^-.

Keywords: Fluorescence sensor, pyrimidine-based probe, binding constant

OP-06

ESIPT triggered turn-on fluorescence probe for rapid detection of highly toxic warfare agent (Phosgene): Strip based real time monitoring of phosgene vapour

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Rapid detection of toxic warfare agent phosgene was achieved by ESIPT triggered turn-on fluorescent probe. The probe was designed by forming imidazole from diamino naphthalene and 2-hydroxy naphthaldehyde it favours ESIPT that makes it fluorescent in DMSO solvent medium. Due to the ESIPT the reaction between phosgene and imidazole happens rapidly and forms new fluorescent molecule with few seconds of addition. The probe can detect upto Nano molar level with LOD 29 nM. Sensitive and quick response of the probe makes it effective towards real time monitoring of phosgene. Eco friendly test strips were made with filter paper and treated with probe to detect phosgene vapour. The strips yield immediate response with phosgene and makes turn on fluorescence within few minutes of reaction time. The probe can be an effective candidate for the detection of toxic phosgene in real time.

Keywords: ESIPT, Phosgene, turn- on fluorescence, strip test, vapour phase detection

OP-07

Copper nanocluster as pH sensor to monitor pH in HeLa cells

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Regulation of pH in living cells are vital to carry out its essential functions and its monitoring in environment is imperative to have a sound ecosystem. Hence it is of vital importance to develop a sensor which can function both *in vivo* and *in vitro*. Herein we have synthesized a tryptophan capped copper nanoclusters using ascorbic acid as reducing agent by high temperature synthesis method. The synthesized cluster was well characterized with UV-Vis, Fluorescence spectroscopy and HRTEM. The cluster was found to be highly emissive under acidic conditions while it undergoes quenching on increasing pH. The change in emission is due to aggregation of clusters which was confirmed by DLS. The synthesized cluster exhibit high stability under stringent conditions thus it was successfully employed in imaging HeLa cells under different pH 3, 7 and 9.

Keywords: Copper nanocluster, imaging, pH sensors and Aggregation.

OP-08

Spectroscopic, cytotoxicity and molecular docking studies on interaction between 2, 4-dinitrophenyl hydrazine derived Schiff bases with bovine serum albumin

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Three new 2,4-dinitrophenyl hydrazine derived Schiff bases (E)-1-(2,4-dinitrophenyl)-2-(n-nitrobenzylidene)hydrazine (where, n = 2, **L1**; n = 3, **L2** and n = 4, **L3**) were synthesized and characterised by FTIR, ^{1}H NMR and mass spectra. The interaction of the ligands (**L1-L3**) with the protein BSA was investigated by fluorescence spectroscopy and molecular docking methods. The fluorescence titration experiments of BSA resulted fluorescence quenching with the incremental addition of the ligands (**L1-L3**). The fluorescence quenching is static in nature and the estimated Stern-Volmer constants of the ligands with BSA followed the order of **L1** ≈ **L3** > **L2**. The modes of binding of the ligands with BSA were explored by molecular docking analysis. In addition, the cytotoxicity of the ligands was examined in live HeLa and HT-29 cells. The IC_{50} values were found in the range 13 µM-243 µM.

Scheme 1. The structures of the Schiff bases **L1-L3**.

Keywords: Schiff base; Protein-ligand interaction; Molecular docking; Cytotoxicity.

OP-09

Micellization and clouding phenomenon of cationic Conventional and Gemini surfactants in aqueous single and mixed systems with EO-PO-*based* star-block copolymer T1304

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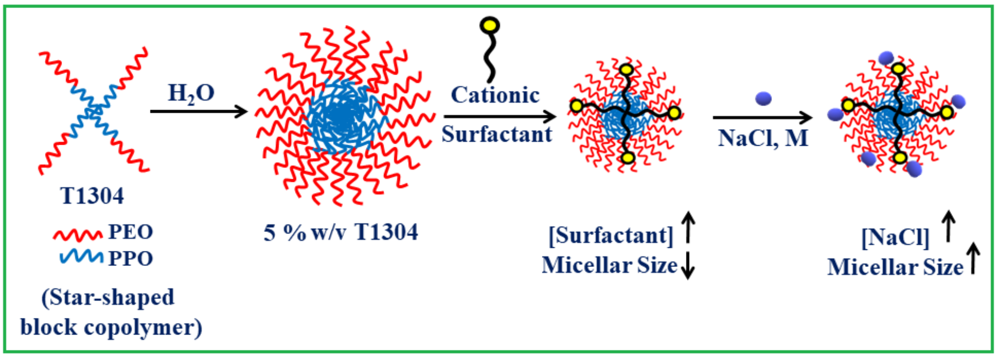
Mixtures of the amphiphilic block copolymers with cationic surfactants find numerous applications in the field of food, pharmaceuticals, cosmetics and detergency. To understand the interactions between them, we herein report the micellization study on the mixtures of a poly(ethylene oxide)-poly(propylene oxide) (PEO-PPO) star-block copolymer, Tetronic®1304 (T1304) with several cationic conventional and Gemini surfactants (GS) using the plethora of physicochemical techniques. The results indicate strong interactions of T1304 with GS in comparison to the conventional analogues with similar alkyl chain length. The presence of cationic surfactants, at lower temperatures, induces micellization. Hence, a significant drop can be noted in the critical micellization temperature (CMT) of T1304. However, in post-micellization regime, the presence of cationic surfactants enhances the surface charge on the copolymeric micelle which leads to the micellar breakdown resulting into the formation of smaller mixed micelles as observed through scattering techniques. The addition of salt, on the contrary, compensated the effect of surfactants and counteracted the hydrophilicity generated in the presence of cationic surfactants.

Keywords: Cationic surfactant, critical micelle concentration (CMC), Cloud point (CP), critical micellization temperature (CMT), hydrodynamic diameter (D_h).



Schematic illustration depicting the micellization and aggregation in 5 %w/v T1304 in aqueous cationic surfactant and NaCl solution environment.

OP-10

Aggregation behavior of stimuli-responsive block copolymers in solution

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Here we report, micellization and phase behavior of a commercially available ethylene oxide – propylene oxide (EO-PO) octablock copolymers, Tetronics® 1304, in the presence of various phenol derivatives as a cosolvents using plethora of techniques such as cloud point (CP), relative viscosity, dynamic light scattering (DLS), and small angle neutron scattering(SANS). The cosolvents with better hydrophobicity displayed improved solution viscosity and increased micellar size while those with low hydrophobicity had an opposite effect.

Keywords: Tetronics® 1304, Cresol, cloud point (CP), dynamic light scattering (DLS), small angle neutron scattering (SANS)

OP-11

Amphiphilic EO-PO star Block Copolymers as Nanocarriers for some Hydrophobic Anticancer drugs

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Commercially available ethylene oxide-propylene oxide (EO-PO) block copolymers are the most studied copolymers for their application in formulations of drugs and targeted drug delivery. The linear EO-PO block copolymers, Pluronics® and their branched analogues Tetronics® have gained enormous attention due to their proficiency to cargo therapeutics and to execute the distribution of the cargo to the site of action. Further, they also improve the pharmacokinetics of the encapsulated drugs and lessen off-target cytotoxicity. Though, a lot of research has been carried out on the linear analogues, a very few studies describing the role of the star block copolymers as nanocarriers has been reported over the years. In view of that, the present study focuses on the role of different additives on the micellization and the release profile of the star block copolymer. It was commonly observed that the copolymers fabricated with longer hydrophilic components showed delayed micellization and poor drug solubilization capacity while those incorporated with longer hydrophobic chains displayed micellization at comparatively much lower temperatures and better solubilization capacity. Although, micellization and solubility of hydrophilic block copolymers can be tuned in the presence of additives. Release profiles exposed slow and sustained release of the drugs from the copolymeric micelles.

Keywords: Block copolymers; micelles; nanocarriers; targeted drug delivery; drug release media

OP-12

Probing the formation of pre-fibrillar prion peptide oligomer with atomistic molecular dynamics simulation

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The structural basis of pre-fibrillar prion peptide aggregation and identification of possible intermediates still eludes us. Knowledge regarding the early stages of fibril formation at atomistic detail may provide suitable information for rational drug design. In this work, using human prion peptide ^{127}GYMLGS^{132} as a model, we studied the oligomer formation process from dimer (O_2) to hexamer (O_6) by employing molecular dynamics with explicit solvent. The results obtained from our study indicate that the oligomer formation initiates from antiparallel β-sheet like dimers. The successive addition of unstructured monomer found to affect the free energy landscape of aggregation. Analysis of free energy profile showed that the conformational transition of the aggregates initiates during tetramer (O_4) formation. The higher order aggregates (O_5 & O_6) found to reorder in to steric-zipper, β-barrel like structures and resides in two energy states separated by small energy barrier. Unlikely, the lower order aggregates (O_2 & O_3) found to remain in single deep minima with extended β-sheet structure. Hydrophobic interaction is found to be key contributor for stabilizing the higher order aggregates and supports the further growth of oligomers. However, the initial association of the monomers is mainly governed by transient interchain hydrogen bonds. The insights obtained from the study will help in understanding the physicochemical forces for the initial formation of toxic prion oligomers.

Keywords: Prion Peptide; Free Energy Landscape; Steric Zipper; β-barrel; Hydrophobic Interaction

OP-13

Amphiphilic dextran and curcumin derived tubustecan nanoarchitecture: A strategy for repositioning the "Red Devil" for effective liver cancer management

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Nanotechnology derived formulations for delivery of anticancer drug is a promising strategy to combat its issues of poor therapeutic performance and severe toxicity. Amphiphilic polymers with tunable size, shape and stimuli responsiveness play a significant role in overcoming the aforementioned challenges. Moreover they can self-assemble into nanoarchitectures of varying morphology thus providing a platform to attain better drug delivery profiles. Biomaterial derived self-assembling polymers are even more promising as effective drug carriers owing to non-toxicity and prolonged blood circulation times. With thisrationale, the present work reports the synthesis and characterization of dextran and curcumin modified amphiphilic polymer that self assembles into tubular nanoassemblies. These tubustecan carriers have been employed for pH and enzyme dual stimuli responsive delivery of DOX.HCl for treatment of liver cancer. The efficacy of this nanoarchitecture as drug carriers has been evaluated "in-vitro" and "in-vivo".

Keywords: Amphiphilic polymers, self-assembly, stimuli responsive, drug delivery, curcumin, biomaterials

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OP-14

Solubilization of Organic Dye in Bile Salt based Surfactants

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In the present work, we sought to probe the aggregation process of bile salt based surfactants. The solubilization of a water insoluble azo dye, Sudan Red G was monitored at a wavelength of 470 nm using a UV-Visible spectrophotometer in presence of two different bile salt based surfactants (Sodium Cholate and Sodium Deoxycholate). The measurements were carried out over a broad concentration range spanning pre and post micellar concentrations. The results indicate that the extent of solubilization of an otherwise water insoluble dye increases substantially with the increase in concentration of both the surfactants. It can be inferred from our investigation that the dye molecules are partitioned in the hydrophobic core of the self-assembled aggregates. The systems investigated involved the use of bio-compatible surfactants derived from renewable source of natural origin, possessing low toxicity, for solubilization of an otherwise water insoluble dye. Such studies offer a green alternative vis-à-vis the existing processes of solubilization that are widely used in textile and other allied industries like imaging, displays, memory technologies, analytical chemistry, indicators for biological sciences, etc.

Keywords: Dye Solubilization, Micelles, Insoluble Organic Dye, Bile Salt based Surfactants.

OP-15

Tensile and Impact Behavior of High Density Polyethylene composites reinforced by Coir fibers and Rice Stalk as Fillers

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Plastic in today's world is creating many problems owing to its non-biodegradability and thus high accumulation in environment. It may be left in the environment as such without being utilized. Also when plastic particles break down, they gain new physical and chemical properties, increasing the risk that they will have a toxic effect on organisms. Plastics do not undergo degradation, thus, stay in the soil for many years, which affects soil fertility and degrades the soil quality. A technology to recycle plastic is called Plastic Waste Management and it is beginning to get attention in lot of countries. Plastic Waste Management deals with the three ways of managing plastic: Reduce, Reuse and Recycle. The present study focuses on Recycle of waste plastic. One such plastic is High Density Polyethylene (HDPE). It is used as a matrix to make composites which is reinforced by Coir Fibers. Filler material being used is the Rice Stalk dust which is otherwise left for burning. Composites were optimized and prepared and tested for Tensile and Impact testing. The composites containing 25 wt% of fibers and 5wt % of rice stalk gave the best results.

Keywords: Plastic, Composite, Properties, Management, Biodegradability.

OP-16

Starch based mechanically tough double cross-linked hydrogel as a toxic metal ion adsorbent

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Hydrogels are one of the most interesting classes of three-dimensional polymeric materials with the ability to absorb a large amount of water and other liquids. These "soft and wet" polymeric materials received utmost importance for numerous applications including controlled-release fertilizer, for enhancement of water holding capacity of the soil, bio-sensor, and adsorbent for wastewater treatment, etc. However, the application of hydrogel as an adsorbent has some shortcomings, including low mechanical strength for which it is troublesome to separate the adsorbent after adsorption and which leads to the source for another water pollution. To overcome this type of problem a hydrogel having the necessary mechanical strength is suitable for easy recovery after adsorption and also helps in the reusability of the hydrogel for the subsequent cycles. Hence, a hydrogel with high mechanical strength was synthesized with a double cross-linking strategy in which starch with epichlorohydrin acts as the first network and acrylic acid cross-linked with *N*, *N*- methylene bis acrylamide incorporated on the starch backbone to act the other network. This synthetic route provides the hydrogel tensile strength of 3 ± 0.3 Mpa and showed satisfactory adsorption capacity for Cu, Ni, and Pb up to three consecutive cycles. It could be expected that the research work provides a new synthetic route for developing a mechanically tough hydrogel with the potential to adsorb toxic metal ions with satisfactory recyclability.

Keywords: Hydrogel, double cross-linking, tensile strength, adsorption, recyclability

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OP-17

Fabrication of bio-based waterborne polyester/ citric acid functionalized reduced graphene oxide nanocomposite as anticorrosive material

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The demanding requirement of environmentally compatible coating materials for metal protection and thereby increasing their durability is drawing substantial research interest. In this milieu, fully bio-based waterborne polyester nanocomposite as an anticorrosive organic coating was fabricated by an environmentally benign route using different renewable reactants and citric acid functionalized reduced graphene oxide as the nanomaterial. Three different compositions of the nanocomposites were fabricated and further characterized by different spectroscopic and microscopic techniques. The thermosets of the resinous nanocomposite were obtained by curing them with glycerol based epoxy and poly(amido amine) as the hardener. The thermosets showed good mechanical properties, thermal stability, corrosion resistance properties (impedance of the order of 10^7ohm cm^2) and biodegradability against *Pseudomonas aeruginosa and Bacillus subtilis* bacterial strains. Therefore, these types of environmentally benign polymeric materials can overcome the shortcomings of petroleum based synthetic polyesters as well as they could be used as a promising high performing anticorrosive coating material for various applications.

Keywords: Sustainable polyester nanocomposite, mechanically tough, biodegradable, anticorrosive.

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OP-18

Structural, Magnetic, Optical and Dielectric properties of Calcium hexaferrite synthesised using Neem and Curry leaves extract

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M type CaM hexaferrite ($CaFe_{12}O_{19}$) are synthesized via green synthesis method using Neem Leaves (Azadirachta indica) and Curry Leaves (Murraya koenigii). They were subsequently given heat treatment and calcination was done at 950°C. FTIR spectra confirmed the formation of Fe-O bond of hexaferrite nano particles. XRD pattern reveals the formation of hexagonal phase of the synthesized particles. Magnetic behavior was studied at room temperature using vibrating sample magnetometer. Optical properties were studied by UV–VIS-NIR study. Dielectric measurements were carried out at room temperature in the frequency range 20 Hz to 2 MHz.

OP-19

Lead(II) based Coordination polymers as electrocatalysts for Oxygen Evolution Reactions

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Coordination Polymers (CPs) are promising candidates for various applications in the field of catalysis, magnetism, sensing, gas adsorption/separation, etc. These are widely used now for solving many energy and environmental related issues. Such materials are also used as electro catalyst in energy storage devices, such as metal-air batteries, water-splitting, and fuel cells. In this work, three coordination polymers based on the room-temperature self-assembly of an earth-abundant metal, Pb(II), a polypyridyl hexadentate ancillary ligand (N,N’N’’,N’’-tetrakis-(2-pyridylmethyl)-1,4-diaminobutane (tpbn))and acetylene dicarboxylic acid (H_2adc) orfumaric acid (H_2fum) or succinic acid (H_2succ) are reported:$[Pb_2(tpbn)(adc)_2].4H_2O\}_n$ (**1**), $\{[Pb_2(tpbn)(fum)_2].5H_2O\}_n$ (**2**) and $\{[Pb_2(tpbn)(succ)_2]\}_n$ (**3**). All compounds are fully characterized byelemental analysis and FTIR Spectroscopy. Their thermal stability is determined by thermogravimetric analysis. Their three-dimensional structures were determined bysingle-crystal X-ray diffraction. Compound **1** is conductive and highly stable in alkaline and neutral medium. It was utilized as anelectro catalystfor Oxygen Evolution Reactions (OER) relevant to energy storage devices, such metal-air batteries, fuel cells and water-splitting.

Keywords: coordination polymer, energy storage, OER, electrocatalyst, thermal stability.

OP-20

Synthesis and CO_2 Absorption Studies of Ionic liquid in a Foam-Bed Reactor

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This research presents the development of a low-cost Protic Ionic Liquid (PIL) for CO_2 gas absorption from a post-combustion system. The PIL was synthesized by proton transfer from Bronsted acid to Bronsted base. The structures of the synthesized protic ionic liquid were elucidated using FT-IR, ^{1}H NMR, ^{13}C NMR, and mass spectroscopy. The present work also examined the CO_2-absorption in aqueous solutions of [TETA] [Lactate] in a foam-bed reactor (FBR). Experimental results show that in foam- bed reactor the synthesized PIL, i.e. [TETA] [Lactate], shows higher CO_2-absorption rate. The effect of surfactant used on the overall mass-transfer coefficient in the absorption process was also determined experimentally. In addition, the effect of different operating variables like types of surfactant, surfactant concentration, lean gas flow-rate, CO_2 flow-rate, the height of foam-bed, and initial concentration of [TETA] [Lactate] upon the volumetric mass-transfer coefficient and subsequently, on carbon-dioxide absorption rate were studied. The carbon-dioxide absorption rate obtained in a bubble-column reactor has been compared with that of a foam-bed reactor. Up to 18% higher absorption rate is obtained in a foam-bed reactor.

Keywords: CO_2 absorption, Lean gas, Surfactant, Foam-bed reactor, [TETA] [Lactate]

OP-21

Study of structural, magnetic and dielectric properties of copper substituted lead hexaferrite synthesized using co-precipitation technique

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M-type lead hexaferrite $PbCu_xFe_{12-x}O_{19}$ (x = 0.0, 0.2, 0.4, 0.6, 0.8 and 1.0) were synthesized by co-precipitation method and heated at 1150° C for 5 hrs. All heated samples were characterized by Fourier Transformed Infrared Spectroscopy (FTIR), X-ray diffraction (XRD), VSM and low frequency dielectric measurements. The presence of two absorption bands in the wavenumber range of 600–550 cm^{-1}and 450–400 cm^{-1} in Fourier transform infrared (FTIR) spectra confirmed the ferrite formation. From x-ray diffraction (XRD) analysis confirms that formed $PbFe_{12}O_{19}$ hexaferrite possesses a major M-phase along with the secondary phase of PbO, whereas copper-substituted samples show the presence of mixed phases: M-phase, α-Fe_2O_3, Pb_3O_4, Pb_2O_3, $CuFe_2O_4$, and PbO. The saturation magnetization of all samples was found to be in the range of 36.22–13.24 emu/g, and the value of coercivity lies in the range of 8 kA m^{-1} to 27 kA m^{-1}. The formed ferrites are magnetically soft with remanence magnetization < 6.5 emu/g. The Cole–Cole-type plots illustrated a single semicircle arc due to the contribution of grains and grain boundaries in prepared hexaferrites, which indicate the resistive properties of prepared materials.

Keywords: M-type, Pb-Hexaferrites, M-type, FTIR, XRD, VSM, Dielectric properties

OP-22

Gasoline desulfurization using modified *Pongamia pinnata* biomass

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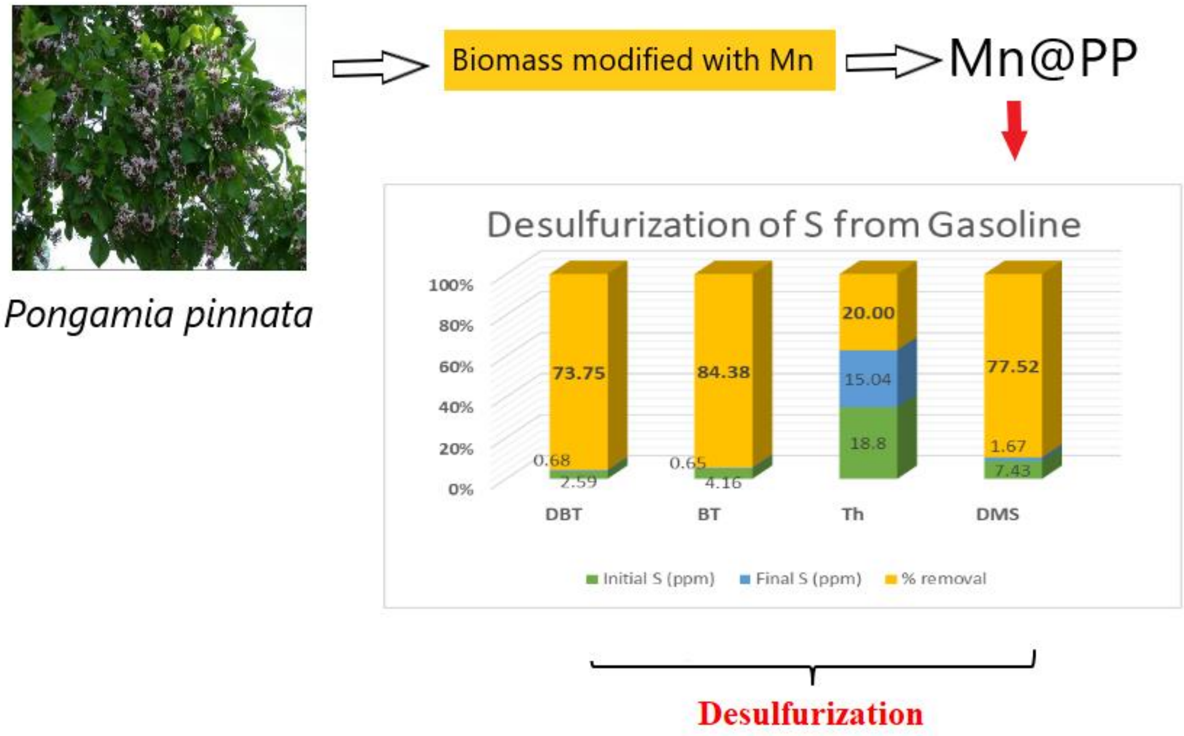
Desulfurization is an essential step in the petroleum refining process due to the environmental effects and health hazards of burning fossil fuels in the transportation sector. SOx is a notorious pollutant resulting from the combustion of transportation fuels and due to the stringent norms being imposed recently to lower the sulfur content below 10 ppm, has compelled researchers to develop new strategic approach besides the conventional Hydrodesulfurization process (HDS), which operates at high temperature, pressure, specialized catalyst under hydrogen flow. HDS is also known to be cost-intensive and less useful for targeting thiophenic sulfur compounds. We have developed a novel adsorbent through manganese modification of activated carbon developed from *Pongamia pinnata* biomass in the present work. Desulfurization studies using Gasoline obtained from an Indian supplier showed the efficiency of the modified porous material. Manganese modified activated carbon could remove ~ 84 % of benzothiophene, 76 % of dimethyl sulfide, and 74 % of dibenzothiophene. The adsorption equilibrium data for desulfurization was investigated using a Gas chromatograph coupled with an FPD detector. The study gave promising results for the potential application of the material for industrial application.

Keywords: Desulfurization, Liquid Fuels, Adsorption, sulfur


Pongamia pinnata
Biomass modified with Mn
Mn@PP
Desulfurization of S from Gasoline
100%
80%
60%
40%
20%
0%
73.75
0.68
2.59
84.38
0.65
4.16
20.00
15.04
18.8
77.52
1.67
7.43
DBT
BT
Th
DMS
🟩 Initial S (ppm)
🟦 Final S (ppm)
🟨 % removal
Desulfurization

OP-23

Effects of torrefaction on physicochemical properties of agricultural residues

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Torrefaction is a promising thermal pretreatment to upgrade the physico-chemical properties of biomass for fuel production. This study presents the results of parametric optimization and characterization of oat hull, canola hull, and barley straw after torrefaction. Torrefaction was conducted at temperatures in the range of 220-300°C and residence times of 30-60 min in a fixed bed reactor. The influence of the operating temperature and time was analyzed to determine optimal operating parameters. The characteristics of torrefied biomass were analyzed by different characterization techniques such as Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Solid-state ^{13}C nuclear magnetic resonance spectrometry (^{13}CNMR) and X-ray photoelectron spectroscopy (XPS) while the morphology of the sample was analyzed by Scanning Electron Microscopy (SEM). Additionally, mass loss, energy yield, higher heating value, enhancement factor were investigated. The highest heating value (25.3 MJ/kg) was found for canola hull followed by oat hull (23.3 MJ/kg) and barley straw (22.9 MJ/kg) at most severe torrefaction condition (300°C and 60 min). The results show that torrefaction significantly boosted up fixed carbon content, fuel ratio, moisture adsorption rate, and decreased volatile matter, the atomic ratio C/H, C/O, cellulose crystallinity for all samples. TGA and DTGA analysis demonstrated that the thermal stability of all feedstocks enhanced noticeably as torrefaction temperature and time increased. The optimum torrefaction conditions were found to be 260°C and 60 min for oat hull and barley straw and 300°C and 30 min for canola hull from an energy point of view. The results from the analysis indicate that torrefaction temperature plays the most dominant role in the properties of torrefied biomass than residence time.

OP-24

Evaluation of Physico-chemical characteristics and scaling Indices of ground water quality of coastal villages of Hansot and Ankleshwar talukas of Bharuch district, Gujarat, India

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Study on the ground water quality was carried out among the coastal villages of Hansot and Ankleshwar talukas of Bharuch district, Gujarat state, India in the year 2018-2019. Ground water samples were collected from 40 different sampling stations of coastal villages of Hansot and Ankleshwar talukas of Bharuch district and were analyzed for their physico-chemical characteristics and different indices for corrosion. The results were evaluated using the standard analytical procedure of APHA (2005). On the basis of evaluation the uses of groundwater for drinking purpose, agriculture as well as industrial was decided. Physico-chemical parameters like pH, TDS, TH, Ca Hardness, Mg Hardness, Ca as Ca^{++}, Mg as Mg^{++} and corrosion indices like Langelier Saturation Index, Ryznar Stability Index, Puckorius Scaling Index and Larson Scold Index were calculated by standard methods. By comparing the results against drinking water quality standards laid by Indian Standards, it is found that most of the water samples are non-potable for human being due to high concentration of one or the other parameter. Most of samples have TDS, TH, Chloride values higher than the permissible limit prescribed by IS. Even at some places corrosion indices are found higher too. The higher values of these parameters may have health implications and therefore these need attention. From different indices it is summarized that water samples at many places have corrosion tendency. So from these locations water should be given pre-treatment before using it for cooling water and boiler purpose.

Keywords: Ground water, Physico-chemical parameters, Corrosion indices, LSI, RSI, PSI, Larson Scold Index.

OP-25

Giant Tetrahedral Cryptands as Cation-Anion Dual Chemosensors

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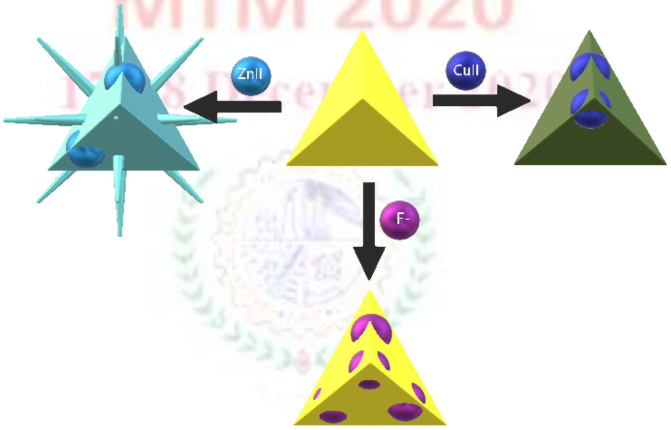
Cryptands are polycyclic host molecules which are capable of encapsulating the guest ions or molecules in the pre-organized cavity depending on steric and interactional complementarities. If cryptands are made up of chromophore/ fluorophore, the binding of ions may result in the change in colour or fluorescence of the solution of cryptands. The property of change in color or fluorescence makes them suitable for development of colorimetric or fluorescence chemosensors.

We synthesized cryptands from bis-salicylaldehyde derivatives and tris-(2-aminoethylamine) under high dilution conditions. The crystalline product was found to be tetrahedral shaped, [4+6] cyclocondensed cryptands as revealed by the single crystal analysis. The structure of cryptand was also retained in the solution state which was confirmed by 2D NMR. The cryptands are capable of binding transition metal ions, heavy metal ions and anions. They are promising candidates for development of colourimetric or fluorescence chemosensors.

Keywords: Chemosensors, Cryptands, Sensor



OP-26

Cyclometalated Luminescence Iridium(III) Complexes

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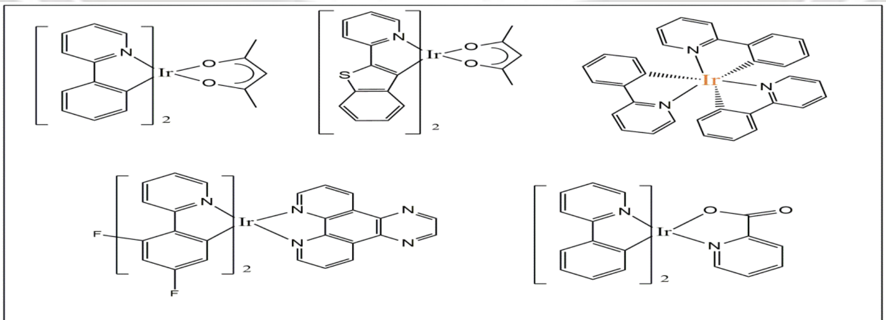
Iridium complexes have drawn attraction due to potential application in various fields Cyclometalated. Iridium complex have been widely synthesised and screened for various properties in recent years. They have been widely used as chemosensors, photooxidants, photocatalysts, sensitizers, bioimaging and anticancer drugs etc.

Phosphorescent iridium (III) complexes have been commonly used as light emitting material in common organic light-emitting diodes (OLEDs) due to their high quantum efficiency. [1]They show various range of tunable light emission by different type of attached ligands. [2] The strong spin-orbit coupling induced fast intersystem crossing (ISC) causes iridium complex as luminescence materials. Phosphorescence emission is caused by mixed excited triplet states i.e. LC and MLCT. Now a days it has become a challenging task to bring quantum efficiency to unit at room temperature in the field of inorganic photochemistry. So far iridium complexes having 12.3% external quantum efficiencies have been reported by some groups.



Some cyclometalated luminescence Iridium complexes

Keywords: Iridium (III) Complexes, Luminescence, quantum efficiency

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OP-27

New Urea derivative for Fluoride anion recognition and sensing

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Over last couple of decade small molecule anion sensing development studies have gained remarkable attention. Mainly, the development of colorimetric anion sensing is even more important and increasingly appreciated since naked eye detection can offer qualitative and quantitative information. It is of great importance to recognize anionic pollutants in the environment along with industrial process. Moreover anion sensing plays important role in biology. Hydrogen bonding sensors are acclaimed in recognizing variety of anions. Therefore, molecules having urea, thiourea, amides, imides are studied widely to obtain sensing of variety of anions. Among all anionic analytes fluoride ions recognition is of much importance as it used in industries, water pollutants, diagnostic and therapeutic medicine for dental care, treatment of osteoporosis, etc.

Here, in present study we have synthesized a molecule having urea moiety which particularly recognizes fluoride anion in presence of other anions. We have synthesized urea derivative from anatharacene-9-carboxylic acid and 2-aminothiazole. The synthesized compound is fluorescent active and gives visible change on fluoride sensing. The compound was characterized by various physico-chemical techniques.

Keywords: Urea derivative, fluoride anion, sensing, fluorescence active

OP-28

Synthesis, solvatochromic and metal sensing properties of N, N′-dimethylvioluric acid

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Heavy metal ions contamination in both living and ecosystems are major public health concerns worldwide. The metal ions enter into the aquatic ecosystem through many spontaneous and human activities. In living systems, heavy metal ions (Cr, Mn, Fe, Cu, Cd, Hg, Pd, and As etc.) are causing numbers of diseases like Minamata, ita-ita, arsenicosis, mental retardation, Wilson’s diseases etc. The detection and removal of heavy metal ions are one of the major challenges for researchers. Violuric acid is one of the most coordinating compounds with polydentate coordination mode. It is a strong field ligand and stabilises the metal complex through the accepting the electron density from metal. Violuric acid and its derivatives helps to identify and determine the metal cations. The pyrimidine ring of the violuric acid derivatives have H-bond donor, H-bond acceptor and pi-stack interaction sites. It has a good ligating property to bind with the heavy metal ions. In the present work, we have reported the synthesis, solvatochromic and metal binding sensing properties of N, N’-dimethylvioluric acid. From our present studies, we are found that N, N’-dimethylvioluric acid is able to sense the Cu^{2+}, Fe^{3+}, Ag^{+} and Cd $^{2+}$ metal ions. The LOD and LOQ value also found low as compared to other reported literatures. Finally, we believe that violuric acid and its derivatives may be used as a sensor for the detection and removal of heavy toxic metal ions in aqueous environment.

Keywords: Violuric acid, solvatochromic properties, sensing properties, LOD & LOQ values.

OP-29

Live-cell imaging of nucleolus and mapping mitochondrial viscosity with a dual function fluorescent probe

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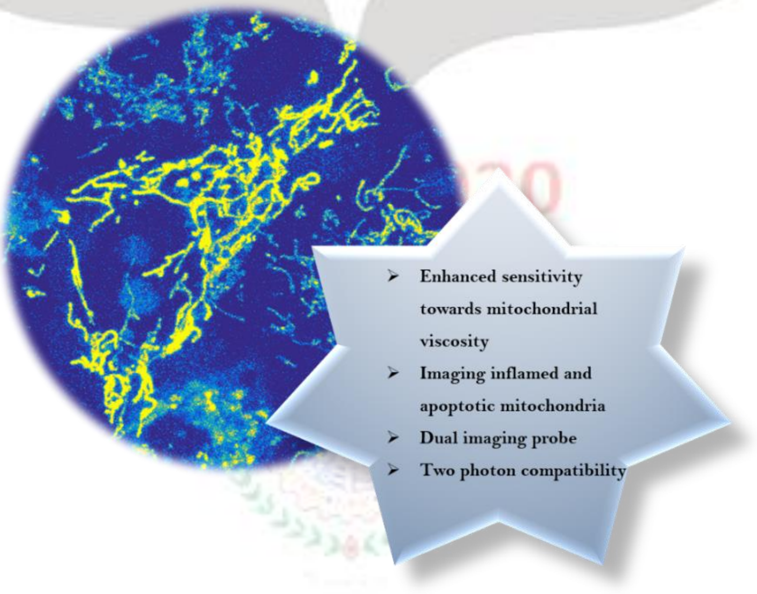
Visualization of various cellular organelles allows determination of several cellular processes and underlying mechanisms. In our work, we report a two photon sensitive fluorescent probe, bearing push-pull substituents and emitting at red region. Its extraordinary responsiveness towards micro-viscosity changes makes it unique than the other existing reporters. Additionally, this also shows specificity in cellular imaging with minimum cytotoxicity. The probe exhibits dual imaging of mitochondria and nucleoli and maps mitochondrial viscosity in live-cells. The impact of mitochondrial viscosity alteration in several pathophysiological conditions is well-known but there is lack of probes to visualize these processes. With the help of our probe, we are able to demonstrate the alteration of mitochondrial viscosity under various physiological conditions such as apoptosis and inflammation. Furthermore, nucleolar staining is confirmed by the RNase digestion experiment to establish its site preferences inside nucleus.

Keywords: Mitochondria, Viscosity, Cytotoxicity, Apoptosis, Inflammation, Nucleoli and RNase.



OP-30

Solvent controlled colorimetric sensing of Cu^{2+} and Fe^{2+} by naphthylamino-glucofuranose conjugate

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Among the various biologically important metals, copper is the third-most abundant metal found in the human body and takes part in many biological processes and enzyme-catalyzed reactions [1]. On the other hand, Fe^{2+} can also play a very crucial role in the biochemical process at the cellular level, such as oxygen metabolism, electron transfer in enzymatic reaction and DNA-RNA synthesis [2]. Considering the above facts, the development of simple colorimetric sensors for recognition of Cu^{2+} and Fe^{2+} in food, pharmaceutical products and biological samples has an important field of research in supramolecular chemistry.

A multifunctional optical sensor by regulating the selectivity towards metal ions by changing the solvent systems appears to be a particularly important field of research due to its real applications [3]. Several molecules have been designed for the recognition of various metal ions by changing the solvent systems. Recently, we have reported that naphthaldimine-based glucofuranose derivative **1** (Fig. 1) could selectively detect Cu^{2+} in 20% acetonitrile in water [4]. Taking into account the effects of solvent for the selection of metal ions, herein, we have studied the selectivity of **1** towards metal ions in DMSO system. In DMSO system, sensor **1** exhibited colorimetric selectivity towards Cu^{2+} and Fe^{2+}. In the presence of both ions, sensor **1** exhibited remarkable naked-eye noticeable color transform and absorption change (Fig. 1). The existence of **1**-Cu^{2+} or **1**-Fe^{2+} complex in solution has been analyzed by absorption spectroscopy and NMR titration experiments. Limit of detection values of receptor **1** as a colorimetric sensor for Cu^{2+} and Fe^{2+} ions are found to be lower than WHO's suggested values.

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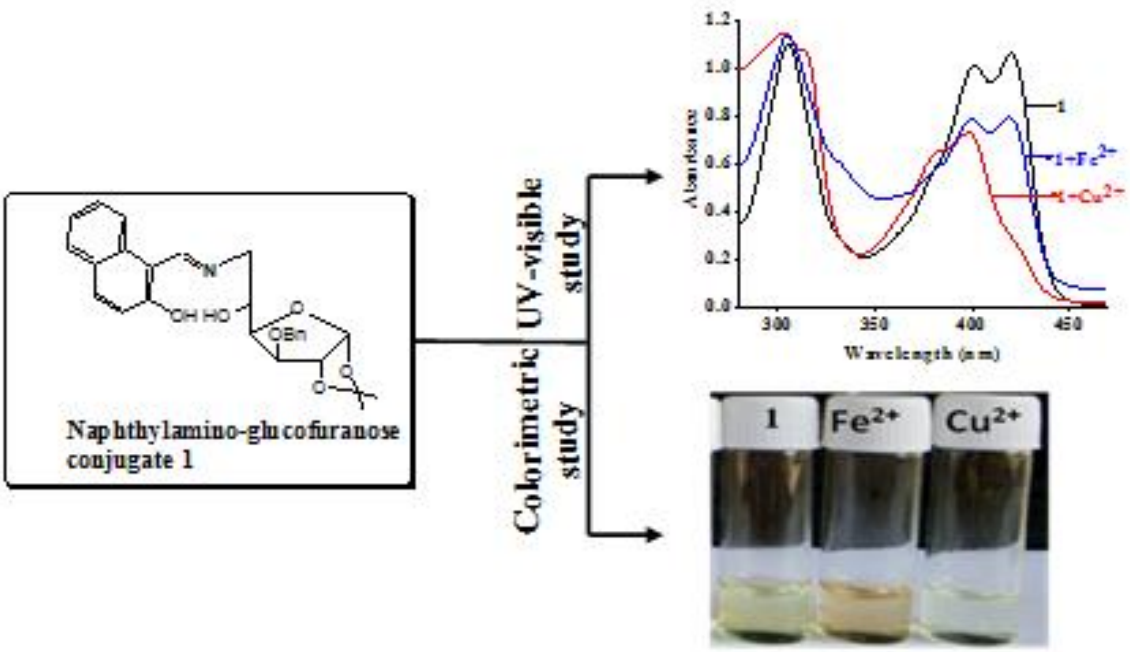

Fig. 1: UV-vis and colorimetric studies of sugar-conjugate **1** with the presence of Cu^{2+} and Fe^{2+} ions in DMSO

OP-31

A C_3-symmetrical tripodal acylhydrazone organogelator for the selective recognition of cyanide ions in the gel and solution phases: practical applications in food samples

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The method of formation of low-molecular-weight organogelators via modifications in the substituents has been demonstrated. The organogelator formed can selectively sense cyanide ions in the gel and solution phases. Interaction of cyanide with acylhydrazone was noticeably visible to the "naked eye" and was proved using ^{1}H NMR titrations. Notably, the ligand has been successfully explored for the recognition of cyanide ions in food samples. Additionally, low-cost cotton swabs coated with the organogelator showed rapid, on-site recognition of cyanide ions. The structure–property relationship discovered in the given study provides insight into the development of novel, cost-effective multifunctional materials.

Key words: Organogelator, Cyanide sensing, Food samples

Reference:

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OP-32

Electrochemical sensing of p-nitrophenol using NiO-NPs-α-CD-rGO modified glassy carbon electrode

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p-nitrophenol (p-NP) is a toxic priority pollutant released from textile industry, leather industry, iron and steel manufacturing, foundries, pharmaceutical manufacturing, rubber processing, and electrical and electronic components production industry [1,2]. p-NP is highly toxic and hazardous due to its high damage capability for the central nervous system, kidneys and liver of human being [3]. Thus, the detection and determination of p-NP present in the environment is an urgent as well as highly important requisite. In this present work, we have demonstrated the stepwise modification of glassy carbon electrode (GCE) surface using reduced graphene oxide (r-GO), α-cyclodextrin (α-CD) and NiO nanoparticles and applied the same for sensing of p-NP. The newly modified electrode was characterized by microscopic and electrochemical techniques. The modified electrode (NiO-NPs-α-CD-rGO-GCE) can simultaneously detect p-NP in presence of o- and m-NP. To quantify p-NP, DPV was carried out within the concentration range of 1-10 μM and found the detection limit of 0.12 nM on the basis of the signal-to-noise ratio S/N = 3 [4]. Interferences of other pollutants such as phenol, p-aminophenol, 4-chlorophenol, 2,6-dichlorophenol and ions like K^+, Cd^{2+}, Cl^-, SO_4^{2-} did not affect the sensing of p-NP. The newly developed sensor had excellent sensitivity, selectivity and reproducibility for the detection of p-NP. The electrode showed good recoveries in river water sample analysis.

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OP-33

Synthesis, Electronic Structure, DNA Binding and Anticancer Activity of luminescent Ruthenium(II)-*p-Cymene* Complexes of imidazo-Pyridine and Quinoline complexes

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Due to severe adverse drug reaction of many anticancer drugs, designing molecules containing more lipophilicity, target-specific, water-soluble, cytoselective and fluorescent properties are highly acceptable. Herewith, we have design and synthesized two new Ru(II)-arene-benzil complexes **Ru-1** and **Ru-2** and analysed by various spectroscopic techniques. The structural studies indication that complex has “piano stool” coordination geometry, consists of one π- bonded arene centroid, two sigma bonded nitrogen atoms from the benzil ligand and one liable chlorine attached to Ru(II). The photo-physical properties of these complexes reveals two absorption peaks are appeared at 230-270 nm and around 400 nm due to involvement of intra-ligand charge transitions (ILCT) and metal-to-ligand charge transitions (MLCT). The binding strength of these complexes with DNA and BSA were found to be 10^5 M^{-1} and 10^3 M^{-1} respectively. The competitive displacement of ethidium bromide (EtBr) from DNA in the presence of these complexes reveals that complex shows an intercalation which is further supported by viscosity and molecular docking studies. The *in-vitro* cytotoxicity test of these Ru(II) complexes were performed with two different cancer cell lines (MCF-7 and HeLa) and their performance were compared with normal kidney cell lines (HEK-293). These experiments revealed that **Ru-1** and **Ru-2** shows the selectivity and potency towards the MCF-7 and both the cancer cell lines (MCF-7 and HeLa) respectively. Here we have observed least IC_{50} value and high selectivity factors in comparison with cisplatin.

Key words: DNA, BSA binding, MTT assay, Molecular docking

OP-34

Colorimetric studies of Aminothienochromene based reactive dyes and their dyeing performance on silk fabric

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A series of hot brand reactive dyes were obtained by the coupling of diazotized naphthalene based acid coupling components with 3-((4-chloro-6-((4-substitutedphenyl)amino)-1,3,5-triazin-2yl)amino) -4H-thieno[3,4-c]chromen-4-one; in good yield. The structure of the synthesized dyes was investigated using FTIR, ^{1}H NMR, elemental analysis and UV spectroscopy. All the synthesized compounds were studied and their dyeing performances as reactive dyes have been assessed on silk fabric. The percentage dye bath exhaustion and fixation on silk fiber was found to be very good. The dyed fabric showed moderate to good light fastness and good to excellent washing and rubbing fastness properties. Colorimetric data (L*, a*, b*, C*, H*, K/S) have also been investigated.

Keywords: 3-Amino-4H-thieno[3,4-c]chromen-4-one, Exhaustion, Fixation, Fastness properties, Colorimetric studies

OP-35

Utilization of CO_2 for the conversion of epoxides to cyclic carbonates catalysed by metal-free triazine-based high surface area nanoporous material: Heteroatoms driven synergy in the superior performance

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Unprecedented increase in the consumption of fossil fuels for the energy production has led to substantial increase in the CO_2 content in the atmosphere causing “the global warming”, the worst challenge facing this generation. Even with all-out effort put together by most of the developed and developing countries could hardly make an appreciable difference to this deadly effect. Among several approaches explored in the recent time, the carbon dioxide capture sequestration and utilization (CCSU) is considered as one of the most promising that could provide some relief to the management of CO_2, while providing sustainable energy and environmental solutions. In this direction, utilizing CO_2 to make energy and industrially important products can definitely contribute towards the sustainability.

In this research, a heteroatoms (N and O) enriched nanoporous material (MNENP) has been employed as a metal-free organocatalyst in the utilization of CO_2 for the conversion of a series of epoxides to their respective cyclic carbonates with high yield and selectivity. The catalyst MNENP was synthesized by a simple condensation of 2-hydroxy-1,3,5-benzenetricarbaldehyde and melamine under reflux condition using DMSO as solvent. Spectroscopic investigations such as FT-IR, ^{13}C CP-MAS NMR and XPS confirmed the structure, while the textural property (specific surface area of 304 $m^2\ g^{-1}$ and total pore volume of 0.95 $cm^3\ g^{-1}$) was investigated by N_2 sorption analysis. An estimated 32.6 and 3.5% of N and O, respectively, can be expected from the condensation of the framework. The material was stable up to a temperature of 320 °C as investigated by TGA. Nearly spherical agglomerated nanoparticles with size of 30-70 nm were estimated from the FE-SEM and TEM images. An amorphous structure was confirmed from XRD and SAED pattern.

The epoxides such as epichlorohydrin, epibromohydrin, 1,2-epoxy hexane, styrene oxide and glycidyl phenyl ether with substituents varying in their electronegativity were investigated. A milder experimental condition with a pressure of 4 bar CO_2 and temperature of 100 °C was enough to complete the reaction with a reaction time of 20 h. A pressure of even 60 bar was required for such a conversion when similar metal-free catalysts were used. The products obtained after purification by column chromatography are confirmed by NMR and GC-MS. Single product with ca. 100% selectivity and conversion were estimated when epichlorohydrin was used. Although, the epichlorohydrin showed best conversion, all other epoxide substrates also have moderate to high selectivity and conversion. Blank reaction in the absence of catalyst has yielded almost no detectable product when the reaction was carried out otherwise in identical condition. A superior recyclability with retention of 79% of its initial activity after five cycles has further justified the use of the catalyst for the CO_2 utilization. The superior performance of the catalyst could be attributed to the presence of the heteroatoms, N and O, these indeed help in activating the CO_2 and epoxide simultaneously, even without a co-catalyst that is very common for such a conversion.

Keywords: CO_2 cycloaddition, Cyclic carbonate, Heterogeneous catalysis, Organocatalysis, Nanoporous material

OP-36

Optimization of Parameters to Improve the Removal Efficiency of Methylene blue by Novel Ordered Mesoporous Carbon

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It has been over a couple of decades since 'adsorption' is being widely employed as one of the most efficient techniques to treat the effluents from various industries, abundantly loaded with toxic pollutants. It is well established fact that the effluents from industries like paper, textile, etc majorly comprise toxic dyes. Mesoporous carbon, the flagship of mesoporous materials, is extensively used as adsorbent to treat dye-polluted waters. Due to some unavoidable drawbacks of using mesoporous carbons like slow reaction rates and poor adsorption capacity, the focus is now shifted to ordered mesoporous carbon, owing to their extra-ordinary properties like high surface area, tuneable textural properties and narrow pore size distribution. Besides the inherent properties of adsorbent, the conditions of adsorption or the factors that have an inevitable role to play in the process of adsorption need to be studied and optimized. Under the present study, the adsorptive potential of a novel ordered mesoporous carbon (OMC) material for a cationic dye, Methylene blue was examined and the effect of various parameters on the adsorption process was studied. The medium pH determines net surface charge of the adsorbent which thereby influences the interactions between the adsorbate and the adsorbent. The study of effect of adsorbent dosage, initial dye concentration and time of exposure are related to the availability of active sites, concentration gradient across solid-solution interface and attainment of equilibrium, respectively. The values of various parameters for the adsorption of Methylene blue over OMC were found as pH=7.0; adsorbent dosage 10 mg/20mL; initial dye concentration = 5×10^{-5} M; contact time= 1 hour 45 minutes. Thus, it can be safely concluded that during the batch adsorption studies OMC was found to adsorb almost 100% Methylene Blue dye.

Keywords: Adsorption, Ordered Mesoporous Carbon, Methylene blue, Solid-solution interface, Dye removal.

OP-37

Role of Interfacial Mixing Zone in T-shape Microchannels of Different Aspect Ratio

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Microfluidic technology generates a platform to modulate fluids in microscale channels has found broad applications in biochemical engineering, which is exemplified by the multiplexed detection of biomarkers and the precise manipulation of cell behaviours, from the individual to the collective. In recent time this platform showed emergence and explosion as alternative routes for chemical synthesis toward both materials and molecules.

Microfluidics has two special characteristics in order to improve chemical synthesis (a) mixing and mass/heat transport in very short time (b) precise control down to µm to nm levels. In microfluidics system fluids are flowing in a very confirmed region by miniaturized micro reactors like microchannels, microtubes, microdroplets, microinterfaces and more important biological cells. Mixing in microfluidic devices occurs at extremely low Reynolds number (Re <100) of laminar microfluidics in a straight channel with micrometer dimensions, where mixing mainly occurred due to molecular diffusion at the interface and requires a long flow path to achieve desired mixing.

The influence of interdiffusion mixing zones for co-flowing streams in microchannels has been studied under various conditions. Two miscible streams (liquid dye samples and deionised water) flowing parallel to each other under laminar flow conditions formed a dynamic/moving interface at the centre of the microchannel. The interdiffusion mixing zone width was measured when it became stable. Results of diffusion dominated mixing zone showed that small changes in flow rates may have displaced the position of the mixing zone and increased for both increasing and decreasing flow rates. It was found that the improvement in the width of the mixing zone is related to flow rates of the streams and geometry of the microchannels.

Microfluidic offers an ideal interface to connect synthetic chemistry with a number of existing technologies that are leading worldwide revolution in the area of 3-D printing, big data and interfacial intelligence. There are large number reviews available online related to this technology but we have broken the landscape of micro-synthesis into two separate aspects, compounds and materials, and provide the platform for the readers with the comprehensive overview of promising technology.

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OP-38

Effect of Substituents on Stability and Antioxidant Activity of Diaryl Selenides and Spirodiazaselenuranes

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Spirodiazaselenuranes are structurally interesting compounds, whose stability highly depends on the nature of the substituents attached to the nitrogen atoms. Aromatic substituents are known to play important roles in stabilizing the Se-N bonds in spiro compounds. In this study, several amino acid substituted spirodiazaselenuranes are synthesized by introducing amino acids substituents to understand their effect on the stability of the Se-N bonds and the antioxidant activity. As per our previous studies aromatic and benzyl shows significant activity. Herein, the replacement of aromatic, benzyl substituent by amino acids shows interesting antioxidant activity.

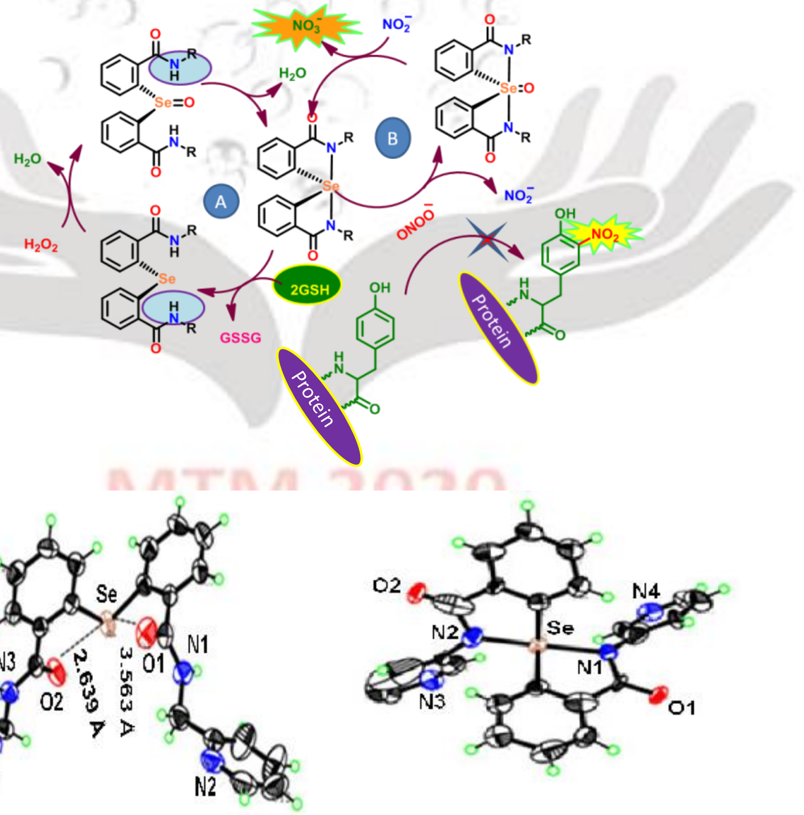

Figure-1: Proposed mechanism for the catalytic cycle of GPx and peroxinitrite oxidation and single x-ray structure of diaryl selenides and spirodiazaselenuranes

Comparison of the glutathione peroxidase (GPx) mimetic activity of the compounds showed that the diaryl selenides having amino acids, heterocyclic rings are significantly more active due to the facile oxidation of the selenium/sulfur centre. However, the activity is reduced significantly for compounds having aliphatic substituents. In addition to GPx activity, the compounds also inhibit peroxynitrite-mediated nitration and oxidation reaction of protein and small molecules, respectively. The experimental observations suggest that the antioxidant activity increases considerably upon introduction of the aromatic, benzylic and amino acids substituents on the nitrogen atoms.

Keywords: Glutathione peroxidase (GPx), Selenium, Antioxidants, Peroxinitrite Oxidation, Spirodiazaselenuranes.

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OP-39

Metallo-Organic Coordination Assemblies (MOCAs) on Surface and in Bulk: Toward Energy and Environmental Applications

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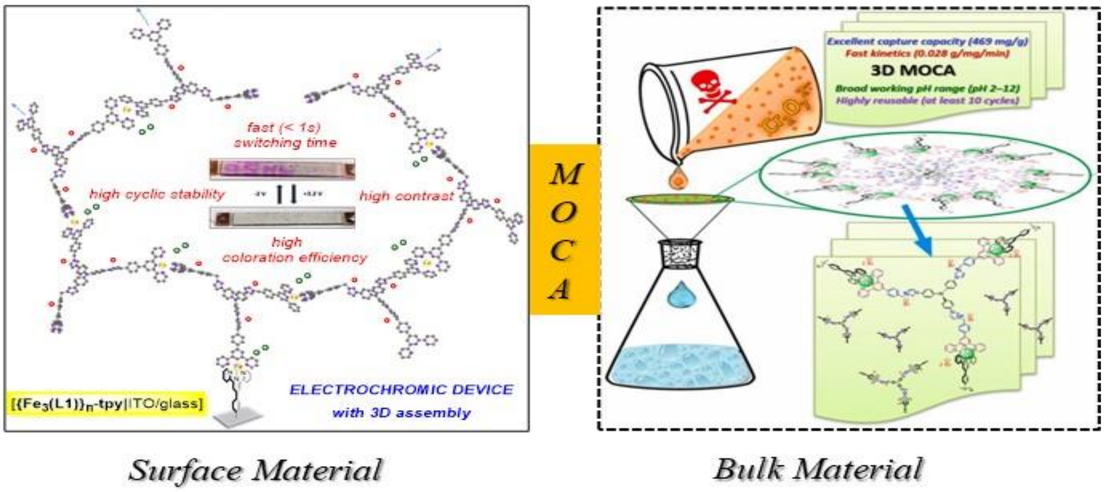
Molecular assemblies (MA) are inherently related to functional nanostructures having a wide range of applications in molecular electronics.[1,2] Therefore, controlled growth of MAs on solid surface is highly significant. Among different techniques, coordination-based stepwise dip-coating method is a promising one for accessing controlled and homogeneous growth of MAs on solid surface. In this context, we have demonstrated a fast (<1 s) switching solid-state electrochromic device (t = 0.49 s for coloration and 0.90 s for bleaching), fabricated with a novel imidazolium-linked $[Fe(terpyridine)_2]^{2+}$ chromophore-based surface-confined three-dimensional (3D) metallo-organic coordination assembly (MOCA) via stepwise coordination of the metal/ligand building blocks.[3] In parallel, the same ligand building block has been utilized with Zn(II) metal ion to synthesize a 3D Zn-MOCA in bulk which was subsequently utilized for wastewater treatment via ion exchange mechanism.[4] In this talk, I'll discuss the key aspects of the molecular design, surface fabrication and the working mechanism of these functional materials.



Keywords: MOCAs, imidazolium, electrochromic, wastewater, Cr(VI), ion-exchange

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OP-40

Synthesis of reduced Graphene Oxide using naturally extracted Tartaric Acid as Reducing agent

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The most emerging and promising field prevailing on present days are the preparation of low-cost and large scale production of materials based on graphene. This research aims at facile and efficient route to synthesize the reduced graphene oxide using the most available natural Tartaric acid/TA from Tamarindus indica as reducing agent. The fabrication of TA-rGO shows high potential in the field of solar application with the enhancement of photocatalytic property. TA-rGO composite formation is confirmed using the X-ray diffraction and Raman spectroscopy.

Keywords: Reduced graphene oxide, Tartaric acid, Tamarindus indica, Photocatalytic property

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OP-41

Fe_3O_4@L-Proline/Pd nanocomposite for one-pot tandem catalytic synthesis of (±)-warfarin from benzyl alcohol: synergistic action of organocatalyst and transition metal catalyst

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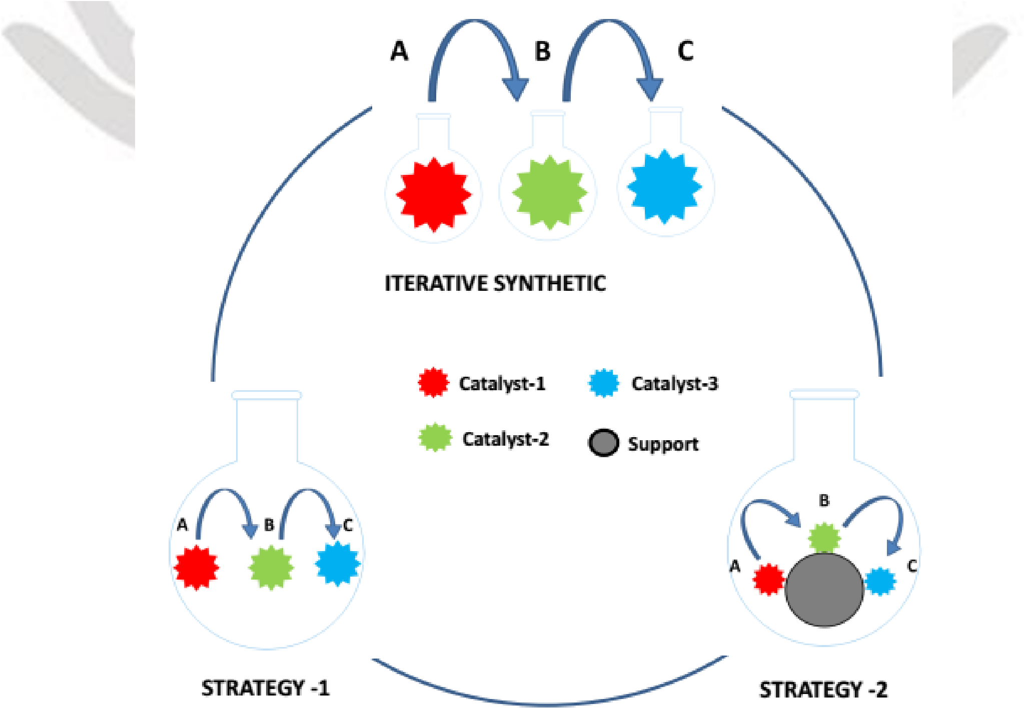
In the current era of organic synthesis, repetitive synthetic strategies are posing serious drawback. Therefore there is a serious need to perform multi-transformations in a single reaction vessel, avoiding the isolation and purification at every stage. One such development is multi-catalysis in which multiple catalytic reactions are done in a single reaction vessel. In multi catalysis system we can have two strategies: 1. there could be different catalysts in a single vessel acting conjunctionally or sequentially, 2.there could be multifunctional catalyst. Scenario 1 is not that lucrative as the isolation of the catalysts in pure form is sometimes not possible or a laborious one. Therefore strategy 2 is the preferential condition.



Here we have developed a one-pot synthesis of (±)-warfarin, an anticoagulant, has been achieved from benzyl alcohol in a 'green way' by using a multicomponent catalyst. For the purpose, L-proline capped Fe_3O_4 nanoparticles (Fe_3O_4@L-proline NPs) were synthesized and metallic palladium was loaded on its surface (Fe_3O_4@L-proline/Pd NCs).

The Pd present on the surface was responsible for oxidation of benzyl alcohol and its derivatives to the corresponding aldehyde *in situ*. This in turn, condensed with acetone to form the aldol condensation product, benzylidene acetone, at 70 °C due to the presence of the L-proline organocatalyst on the surface of Fe_3O_4 NPs. Later, 4-hydroxycoumarin was introduced to condense with *in situ* generated benzylidene acetone by a Michael addition to form the target product (±)-warfarin

Keywords: One pot synthesis, Tandem reaction, PEG 400, Oxidation of benzyl alcohol, Warfarin, Organocatalysis

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OP-42

Production of 5-Hydroxymethylfurfural from microcrystalline cellulose using a Combination of Lewis and Brønsted Acid Catalysts

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The increasing concerns on climate change and the depletion of fossil resources have accelerated dramatic demand for sustainable alternatives and the conversion of lignocellulosic biomass. Lignocellulosic biomass is mainly composed of cellulose, hemicellulose and lignin (constituting 15–30% by weight and 40% by energy) in biomass. It is an amorphous polymer composed of three types of phenylpropane units which holds the most abundant source of aromatic compounds in nature with enormous potential for producing aromatic chemicals and liquid biofuels. However, the complex linkages of side chain and recalcitrant structure of lignin hinder its dissolution and depolymerization. One-pot conversion of lignin using appropriate bronsted and Lewis acids facilitates the extraction of lignin in raw biomass and subsequent degradation of carbohydrates. This approach is a potential lignin-sustainable strategy for its hydrolysis in one pot without separate delignification step. The effectiveness of the Bronsted and Lewis acids for the conversion of glucose to fructose was studied in terms of their intrinsic properties, such as the softness and ionic radius. It was observed that the increased catalytic activity with decreasing ionic radius can be attributed to stronger electrostatic interaction between glucose and the smaller cations, caused by an increase in the effective surface charge density of the ion. Further, pH of the solution plays a key role in controlling the Lewis acidity and Bronsted acidity of the aqueous solution. Therefore, for the conversion of biomass to HMF, the acidic pH is responsible for the formation of the catalytically active species, thus facilitating glucose ring opening and the subsequent dehydration reactions. This study explores the potential of waste biomass towards bio-based chemicals with a focus on commercially viable technologies and provides in-depth insight into the breaking of the intramolecular linkages in lignin could provide an opportunity for the valorization of lignin to obtain high-quality liquid fuels.

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OP-43

Synthesis and Characterization of Graphene oxide using Hummer's Method

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Graphene oxide is the modified form of graphene that consists of oxygen molecules in the form of various functional groups such as epoxides, alcohols and carboxylic acids. It is known for its unique properties of low cost, good scalability to convert into various sizes and shapes and durability to convert back into graphene. The physical, structural and functional properties of the graphene oxide are based on the chemical exfoliation methods chosen for the synthesis. In this research article, we report the synthesis of graphene oxide using Hummer's Method. For the synthesis of graphene oxide, the ice bath set up is made and the concentrated sulphuric acid is mixed with graphite powder to promote the chances of complete exfoliation. The addition of potassium permanganate and sodium nitrate to the above mixture promotes oxidation. Here, hydrogen peroxide is used as a terminating agent to the mixture to terminate the reaction process. The produced mixture had gone under various Characterizations like UV-Vis Spectroscopy and X-Ray Diffraction to observe the formation of graphene oxide. The presence of C=O and C=C bonds were reported using the UV-Vis Spectroscopy where the high intense peak at 233.33nm due to π-π^* transition determines C=C bonds and the peak at 330nm wavelength due to n-π^* transitions determines the presence of C=O bonds. The presence of graphene oxide is reported using the X-Ray Diffraction with a sharp peak is formed at 10.092° diffraction angle. The results from UV-Vis Spectroscopy and X-Ray Diffration shows that the obtained graphene oxide is of high purity with the flake size of 7nm. The synthesized graphene oxide is used for various applications such as Solar Cell Applications, Dyes, Battery Materials, and Biosensors etc.

Keywords: Graphene Oxide, Chemical Exfoliation Methods, Hummer's Method, Graphite Powder, Concentrated Sulphuric Acid, Potassium Permangante.UV-Vis Spectroscopy, XRD, Flake size, Diffraction angle, Wavelength.

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OP-44

Improvement of physico-mechanical properties of fly-ash mortar by using Graphene oxide nano-material

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Graphene oxide nanomaterial can be used as a reinforcing agent in building material to enhance the compressive, tensile strength and durability of fly-ash based cementitious nanocomposites (FCNCs). Common building materials fly ash mortars were reinforced with various amounts of Graphene oxide. Compressive and tensile strengths were improved by a maximum of 35% and 60 % respectively for 0.125% GO incorporated. The standard water absorption should not be greater than 20% of volume; for high-class brick composites, it must be less than 15% of volume. The results show water absorption capacity of fly ash mortar nanocomposites decreases to 13.33% of volume (FCNCs) with the addition of graphene oxide. These results revealed that fly ash brick nanocomposite exhibit excellent durability and low water absorbing ability.

Keywords: Fly ash, Graphene oxide, Compressive strength, Tensile strength and durability.

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OP-45

Molecular docking and structural dynamics strategies validating baloxivir and baloxivir marboxil against SARS CoV-2

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At present SARS CoV-2 emerged as global pandemic and an emergency due to its contagiousness and high mortality. To overcome this problem, the development of novel drugs as well as repurposing of drugs is very much necessary for immediate medication. In this research article we reported molecular docking and GROMACS MD simulations validating the two influenza antiviral drugs baloxavir acid and baloxavir marboxil as therapeutic agents against target proteins of SARS CoV-2, i.e.,3CLpro, PLpro and RdRp. Autodock Vina results of drug candidates baloxavir acid and baloxavir marboxil were analysed and compared. The computational results showing baloxavir acid pose binding affinity towards catalytic sites of Mpro and RNA-dependent RNA polymerase, whereas the baloxavir marboxil only interacts with the active sites of RNA-dependent RNA polymerase. Also, baloxavir acid is binding more effectively at the active site of RdRp than baloxavir marboxil. Hence the molecular docking and molecular dynamic simulations data reveals that the baloxavir acid may be more effective against COVID-19 as compared to baloxavir marboxil.

Keywords: COVID-19; Molecular docking; MD simulations; Anti-influenza drugs; Baloxavir acid; Baloxavir marboxil.

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OP-46

A simple and an efficient protocol to prepare cyclohexanol: Secondary amine catalyzed solvent free diastereoselective cross domino reaction

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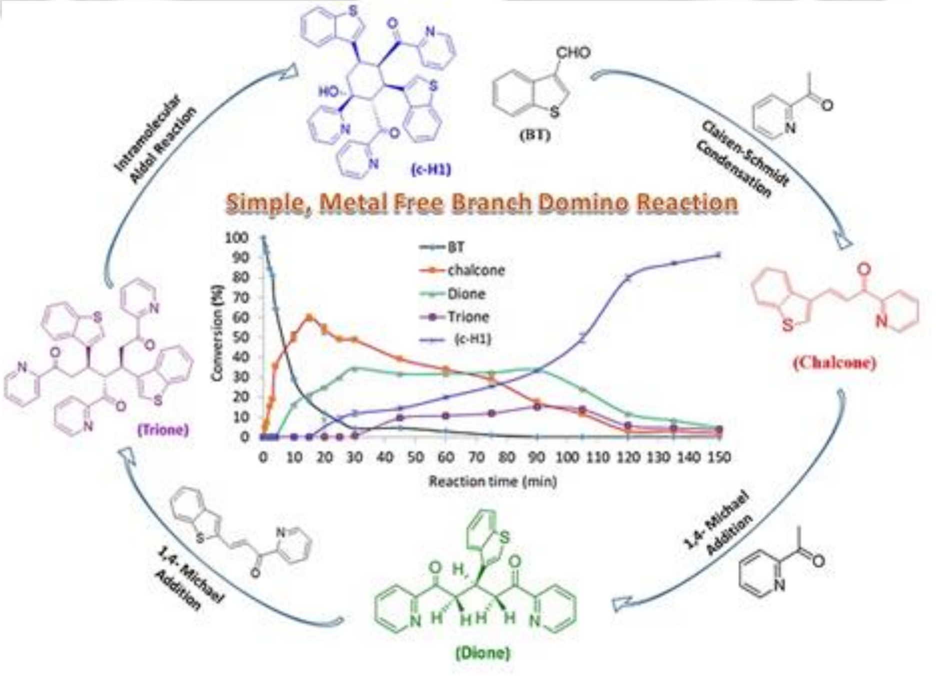
Continues to our earlier solvent based KOH catalysed diastereoselective cross domino reaction, here we are reporting more effective and easier secondary amine catalysed solvent free protocol. A steric hindrance driven diastereoselective cross domino reaction gave manifold heteroaryl substituted cyclohexanols with five asymmetric centers in > 98% yields. The sequence of inter and intra molecular domino reactions are Claisen Schmidt condensation followed by 1,4-Michael addition of heteroaryl carbaldehydes and heteroaryl acetyl derivatives. HPLC study of the reactions shows outstanding self diastereoselectivity (dr > 99%) in the formation of one set of enantiomers out of sixteen possible enantiomeric pairs. The structures of all the synthesized molecules are confirmed by HRMS, NMR and IR spectroscopic techniques. The stereochemistry of the synthesized compounds is established using 2D NMR.



OP-47

Degradation of Azo Dyes from Industrial Influents by Bio Inspired Sustainable Nano Catalysis

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Continues about the application of our earlier reported bio inspired sustainable nano catalyst, here we are reporting more effective and easier protocol for the degradation of azo dyes from industrial waste. Yeast supported gold nanoparticles (CpGNP), prepared by a simple and green method can selectively degrade the azo dyes and various derivatives with different functional groups using sodium borohydride. The product of degraded pure dyes, i.e. aryl amines which are useful for the preparation of pharmaceuticals, polymers and agrochemicals were obtained in good yields (up to >80%) using nano catalyst under mild conditions. The catalyst showed high reusability and is a robust free flowing powder, stored and used after a year without any damage in catalytic activity. The direct treatment of the azo dyes industrial waste is under process. The initial results of the study will be presented during the conference.

Keywords: Bio Inspired, Nano Catalysis, Azo Dyes, Industrial Waste

OP-48

Asymmetric direct aldol reaction in emulsion system: environment friendly concept for chiral induction

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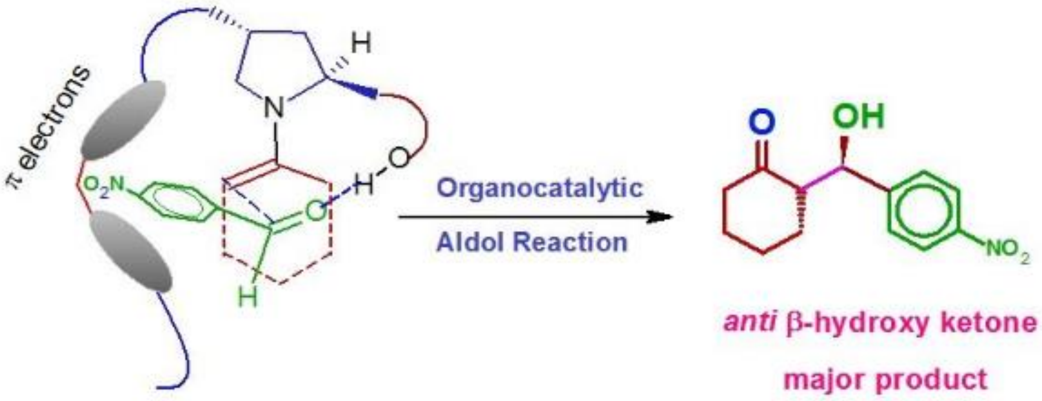
We have demonstrated that chiral induction in the aldol product is possible by generating an enzyme-like cavity in molecular framework of the amphiphilic catalyst. The esters of *trans*-4-hydroxy-L-proline and long chain fatty acids have been synthesized by *O*-acylation. Synthesized molecules were used as catalysts for asymmetric direct aldol reaction between 4-nitrobenzaldehyde and cyclohexanone. The molecular framework of the catalyst not only induces the amphiphilicity but also acquires specific conformation leads to formation of catalytic cavity facilitating stereo-induction in the aldol product. Systematic addition of olefinic bonds in the long hydrocarbon chain makes this cavity more robust stabilizing transition state of the aldol product. By proper tuning of the water content and % loading of the catalyst in aldol reaction, o/w or w/o type emulsion is formed due to aggregation of catalyst molecules. Performance based evaluation of catalytic activity suggests that aldol reaction proceeds with ~ 99% yield, 84% dr and 97.94 % ee in presence of 10% catalyst (having three p bonds), in an o/w emulsion (85 equiv. of water) within 12 h. The stereoselectivity of the catalyst is almost maintained up to 2.5 % loading. The high stereoselectivity of the aldol reaction is maintained even on increasing the amount of water to 300 equiv. A plausible reason has been proposed for retaining the high stereoselectivity and corroborated by computational analysis.



Keywords: Organocatalysis, direct asymmetric aldol reaction, proline, Enantioselectivity, Chiral Induction.

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OP-49

Phytochemicals useful against SARS CoV-2: a search through molecular docking

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From the beginning of the year 2020, the corona virus named SARS-CoV-2 spread globally and this respiratory disease cause the ongoing pandemic. Due to non-availability of recommended medicines and/or drugs for the treatment of COVID-19, in silico computational studies were performed to search repositioning drugs from the different databases and drugbank [1]. In addition to FDA approved drugs, medicinally important phytochemicals are also searched to develop therapeutic approaches. In presentation about the different phytochemicals identified by different groups up to now and suggested for further experimental study. Also, the outcomes of our research on searching phytochemicals with the five protein targets i.e., RNA-dependent RNA polymerase (RdRp), PLpro (Papain like protease), Mpro (main protease), spike glycoprotein (SGp) and SARS-CoV-2 chimeric receptor-RBD (ACE2) of SARS CoV-2. The search is mainly focus on the phytochemicals present in Lycoris species, and observed some phytochemicals binding effectively with the target proteins.

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OP-50

Extraction of phytochemicals from stem-bark of Acacia karroo and evaluation of its Antimicrobial activity

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Acacia karroo which is locally known as Babool is taken for the research. The extraction of Phytochemicals from stem-bark of Acacia karroo was carried out by ultrasound method using Acetone and Methanol as solvents. The Maximum yield obtained 10.25% has been obtained at 40 KHz frequency at 40 °C for 40 minutes in methanol solvent and 9.113% at 40 KHz frequency at 45 °C for 30 minutes in acetone solvent. Phytochemical analysis revealed the presence of Flavonoid, Alkaloid, Steroid, Tannin, Saponnin, Carbohydrate and Gum and Mucilage. Extract prepared in methanol showed good antibacterial and antifungal activity against *B. subtilis*, *S. penumoniae, E. coli* and *S. typhi*; and *C. albicans* fungal strains while moderate in acetone.

Keywords: Acacia karroo, Ultrsound Extraction, Phytochemicals, Antimicrobial activity

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OP-51

Green Route for the Synthesis of Novel Schiff Base 2-((E)-((4-aminophenyl) imino) methyl-4-((E)-(4-chlorophenyldiazenyl) phenol and its Anti-Bacterial Activity

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4-chlorobenzenediazonium silica sulphate was synthesized by taking p-chloroaniline and $NaNO_2$ with silica sulphuric acid as a catalyst. Ultrasound method was used for the Schiff -base (E)-2-(((4-aminophenyl) imino) methyl phenol by taking salicylaldehyde and p-phenylene diamine. The synthesized 4-chloro benzene diazonium silica sulphate and (E)-2-(((4-aminophenyl) imino) methyl phenol was further grinded to obtain the final product 2-((E)-((4-aminophenyl) imino) methyl-4-((E)-(4-chlorophenyldiazenyl) phenol was characterized by Thin layer chromatography and Infra-red spectroscopy and was investigated for its anti-bacterial activity against E.coli and S. Typhi bacteria.

Keywords: Salicylaldehyde, Red-azo dye Schiff Bases, Ultra sound, Grinding, Anti-microbial activity.

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OP-60

Preparation of exhausted coffee residue derived porous carbon-based sorbents for carbon dioxide capture: Effect of surface chemistry and porous structure

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The increased worldwide demand for energy intensifies the combustion of fossil-based fuels with escalated greenhouse gases concentration in the atmosphere. To alleviate the catastrophic environmental scenarios, a quick mitigation effort is required. CO_2 capture and storage (CCS) technology is becoming a very active research area motivated by governments and scientific institutes due to the increasing awareness of global warming. Among the various techniques and processes that have been developed and that are emerging for CCS of CO_2, solid CO_2 carbon-based adsorbents are widely applied. The exhausted coffee residue (ECR) is readily available in large quantities and easy to process without size reduction; it allows the production of biochar via slow pyrolysis. In Canada, coffee accounts for almost three-fourth of the hot drinks market. For each kg of soluble coffee, almost 0.91 kg of spent coffee grounds are generated, then for million tons of green coffee beans (one-fifth of the total worldwide production) the amount of coffee grounds produced is devastating. Thus, this paper intended to demonstrate the complete utilization of ECR to reduce this solid waste and transform it by valorization technique to a value-added product to trap recalcitrant CO_2. This work aims to fundamentally investigate the impact of pyrolysis temperature on the corresponding biochar considered representative for the post-combustion CO_2 capture scenario. Throughout this paper, the biochar ECR which was proposed to be a separation medium for CO_2 capture is evaluated in terms of physio-chemical characteristics, CO_2 breakthrough time (t_B, min) and equilibrium adsorption capacity (mmol/g of biochar). Also, this paper will present the effect of pyrolysis temperature on the surface chemistry and porous structure. The investigation on the enhancement in aromaticity, basicity and surface area of the biochar was confirmed by the FT-IR spectroscopy, Raman spectroscopy, XPS, NEXAFS analysis and BET surface area measurement, which is expected to confer with critical information related to the dynamic CO_2 capture performance.

OP-53

The emerging chemistry of *peri*-naphthoindigo

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*P*eri-naphthoindigo (PNI), with potential applications in diverse areas, is a fascinating dye that contains four different functional groups sandwiched between naphthalene rings (Figure 1).[1] Structure of the dye was proposed first time in a patent in 1977.[2] However, the challenging synthesis was accomplished only in 2018.[1] Unlike its benzene analogue, the famous indigo dye, PNI exists in mono-enol form and exhibits many different properties than that of indigo. The new dye exhibits wider and stronger absorption band than that of indigo with bathochromically shifted maxima (632 nm, in $CHCl_3$). PNI exhibits better electrochemical profile than that of indigo, making the former as better candidate for organic electronics. The same is supported by theoretical calculation as well.[3] Due to distinct structural feature of PNI, the dye shows halochromism upon protonation, marked by red shifted absorption maxima (698 nm). The dye shows aggregation induced enhanced emission (AIEE) phenomenon in appropriate solvent system.[4] However, the most intriguing property of PNI is its ability to install AIEE in other molecule that does not show photoluminescence enhancement alone. Photo and electrochemical properties can easily be tuned either by introducing substitution at the naphthalene ring of PNI or by metal-coordination.

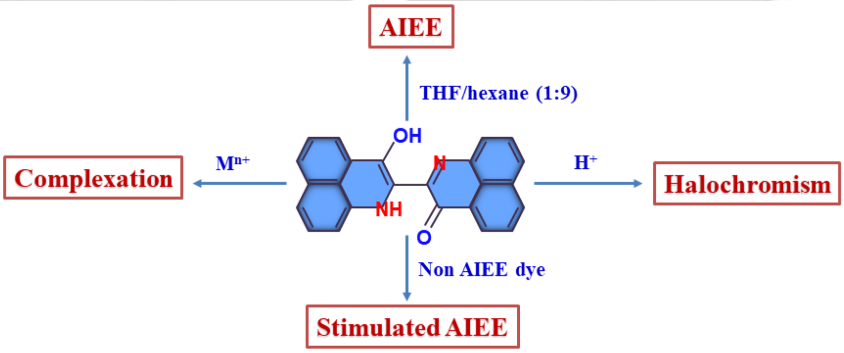

Figure 1. Structure of PNI and its utilities.

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OP-54

Response of Copper based Substrate for Oil-Water Separation under different External Stimuli

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Oil-water separation has become a global challenge due to frequent oil spillage accidents, chemical leakage, or oily waste-water released from industrial activities. To resolve this, issue many approaches/technologies have been used, among them membrane-based technology is attractive for effective separation efficiency. Wettability of separating membrane is an important factor that influences the oil/water separation process, fabricating various membranes with desired wettability can solve this problem. In this regard various substrates have been modified to selectively remove oil or water. One of the promising substrates is copper based such as copper foam, or copper mesh. Such systems have been utilized for oil/water separation application. The separation process can be performed under different conditions to improve efficiency. One of the strategies is to employ stimuli responsive substrate. The external stimuli (i.e. pH stimuli, UV irradiation, thermal stimuli etc.) have been used for separating mesh. The external stimuli switch the surface wettability of the fabricated membrane from super-hydrophilic to super-hydrophobic and vice versa. Hence copper based substrates have found potential applications in oil/water separation.

Keywords: Separation efficiency, Wettability, Stimuli responsive, Superhydrophobic.

OP-55

Naphthalimide-gold-based nanocomposite for the ratiometric detection of okadaic acid in shellfish

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Okadaic acid (OA) is one of the known marine biotoxins produced by various dinoflagellates and exists in seafood such as shellfish. The consumption of contaminated shellfish with OA leads to diarrheic shellfish poisoning (DSP), which results in the inhibition of protein phosphatase enzymes in humans. This poisoning can cause immunotoxicity and tumor promotion due to the accumulation of okadaic acid in more than the allowed limit in bivalve molluscs. The reported methods for the detection of okadaic acid include mouse bioassays, immunoassays, chromatography coupled with spectroscopic techniques, electrochemical sensors and immunosensors. We have developed a naphthalimide-gold-based nanocomposite for the detection of okadaic acid. Individually, the organic nanoparticles (ONPs) of synthesized naphthalimide-based receptors and gold-coated ONPs are less sensitive for detection. However, fabrication of the composite of Au@ONPs and ONPs enhance the sensing properties and selectivity. The composite shows a ratiometric response in the UV-Vis absorption spectrum and quenching in the fluorescence profile with a detection limit of 20 nM for OA in aqueous medium. In cyclic voltammetry, a shift was observed in the cathodic peak (0.532 V to 0.618 V) as well as in the anodic peak (0.815 V to 0.847 V) with the addition of okadaic acid. To study the quick binding of the composite with OA, a time response experiment was performed. Also, the developed sensor retains its sensing ability in the pH range of 5–9 and in high salt conditions. Our developed composite can be used for the detection of OA in real applications.

Keywords: Okadaic acid, toxins, nanocomposite, sensor, naphthalimide.

OP-56

Effect of process parameters on recovery of Lactose from an aqueous solution using PVDF polymer membrane

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The development of high performance and innovative process is crucial for sustainable industrial growth. Membrane science and technology satisfy the requirement of process intensification and lead to significant innovation in both, processes and products. One such technology is membrane distillation. Membrane distillation is a non-isothermal process. Driving force for membrane distillation is a partial pressure gradient across a membrane. A microporous hydrophobic membrane is used for contact between aqueous solutions. In the present work, the PVDF (polyvinylidene fluoride) flat sheet membrane was fabricated to carry out direct contact membrane distillation (DCMD) process. A membrane of different PVDF wt% was prepared. An aqueous lactose solution of varying concentration was used to study the direct contact membrane distillation (DCMD) process. The effect of various operating parameters such as feed temperature, distillate temperature, and feed flow rate was investigated. The effect of these operating parameters on flux and yield of lactose was also investigated. The results show that the increase in feed temperature, feed flow rate and lactose concentration though with decrease in distillate temperature and PVDF polymer wt%, increases the flux and yield of lactose.

Keywords: Membrane distillation, PVDF, and Lactose

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OP-57

Synthesis, Characterization and Electrochemical studies on Citrus limetta (Mosambi) oil, a new Corrosion Inhibitor

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A natural corrosion inhibitor (Citrus lemetta peel oil) has been reported which can be an exemplary replacement of the traditional toxic corrosion inhibitors by decreasing the environmental issues as well as cost. In present scenario, the improvement of green corrosion inhibitors and green inhibition systems are profoundly requested due to the expanding request of green science in the zone of science and innovation. The oil has been extracted from the mosambi peels and tested for its corrosion inhibition efficiency on mild steel (MS) in 1M of HCl medium using Electrochemical methods studies like Potentiodynamic Polarization and Electrochemical Impedance Spectroscopic (EIS). The oil has also been characterized by some physico-chemical studies like Scanning Electron Microscopy (SEM) and Fourier Transform Infrared Spectroscopy (FTIR). Electrochemical studies revealed that it is an efficient corrosion inhibitor showing anodic type of inhibition activity on MS.

Keywords: Natural Corrosion inhibitor, Mild steel, Corrosion inhibition efficiency, electrochemical studies.

OP-58

Precision synthesis of macromolecules using recoverable and recyclable alloy nanoparticle catalyst and their applications

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Stimuli-responsive polymers undergo changes in response to external stimuli (e.g. temperature, pH, light, salt concentration, redox, etc.) Multi-stimuli responsive macromolecules exhibit improved diversity compared to single- or dual-stimuli responsive macromolecules.[1] This is due to their ability to respond precisely to external stimuli. However, till date, the ability of the multi-stimuli responsive polymers to provide the required response-specificity and tunability is still in its infancy. The probable reasons for this are (a) challenging and costly synthesis protocols and (b) the complexity in balancing the various material parameters which includes functionality, reaction feasibility, degradability, hydrophilicity etc.

On the other hand, fluoropolymers are niche products which exhibit unique properties such as exceptional thermal and chemical stabilities, low inflammability, inertness to acids and common solvents, low dielectric constants and dissipation factors. Most of the fluorinated monomers are gas at room temperature and they require special handling. Until recently, only Iodine Transfer Polymerization (ITP)[2] and Reversible Addition-Fragmentation Chain Transfer (RAFT)[3] polymerization allowed some control on the polymerization of fluoromonomer, such as vinylidene fluoride (VDF). To go beyond the limits of the RAFT and ITP of VDF, Cobalt-Mediated Radical Polymerization (CMRP)[4] was also examined. This contribution will present recently developed recoverable and recyclable nickel–cobalt magnetic alloy nanoparticle catalyzed reversible deactivation radical polymerization of vinyl monomers at room temperatures. The catalyst offers multiple advantages such as easier catalyst preparation and handling, predictability, simple recovery and reusability up to multiple cycles without a notable decrease in the control over the polymerization. This makes the process an ideal methodology for the synthesis of smart, functional polymer materials with pre-designed functionalities as a tunable platform to fabricate intelligent materials for emerging applications in materials and biomedical field.

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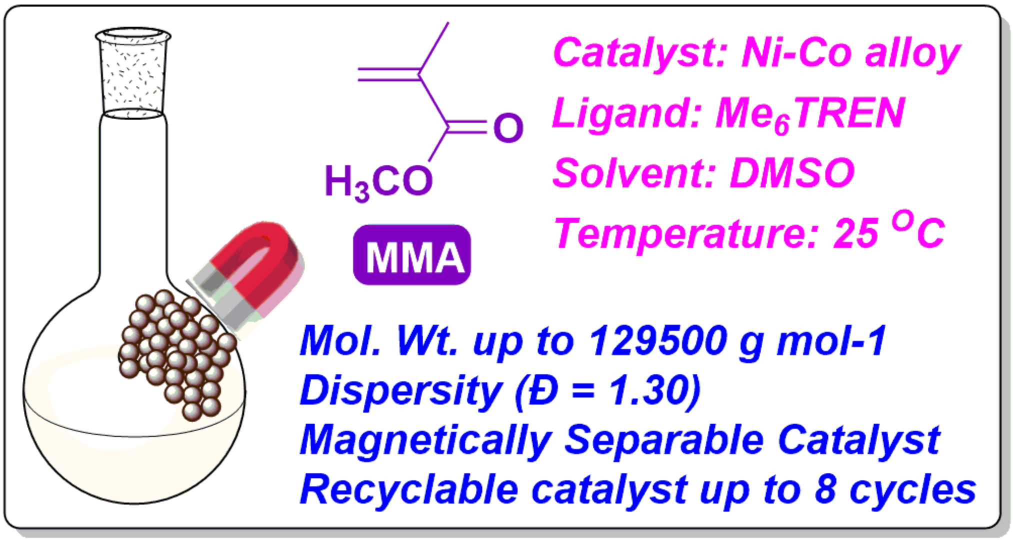

Figure 1: Ni-Co magnetic alloy mediated controlled polymerization of vinyl monomer

OP-59

Environmentally benign synthesis of n-pentyl levulinate via levulinic acid esterification

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In the present endeavor, an environmentally benign process has been investigated to convert levulinic acid into useful chemical. Amongst various zeolites, H-ZSM-5 zeolite was found as most efficient catalyst for the esterification reaction of LA to produce *n*-pentyl levulinate. Further, the catalytic activity of the synthesized material is assessed towards synthesis of n-pentyl levulinate, from biomass derived levulinic acid via esterification reaction. N-pentyl levulinate is one of the value added chemical having wide use as fuel additive, plasticizing agent and fragrance. The presentation will include discussion on comparison of various solid acid catalysts' activity towards the synthesis of n-pentyl levulinate and also the comparison of different alcohols on the synthesis of n-pentyl levulinate via LA esterification reaction. Maximum % conversion of n-pentyl levulinate was realized within 4 h, using H-ZSM-5 catalyst, which is not reported so far. The present green protocol may be useful for the development of efficient procedures to synthesize other value added chemicals from real agricultural residues.

OP-60

Probing the molecular interactions in the binary mixture of choline chloride-based deep eutectic solvent with 1,4-butanediol by the spectral, computational and thermophysical study

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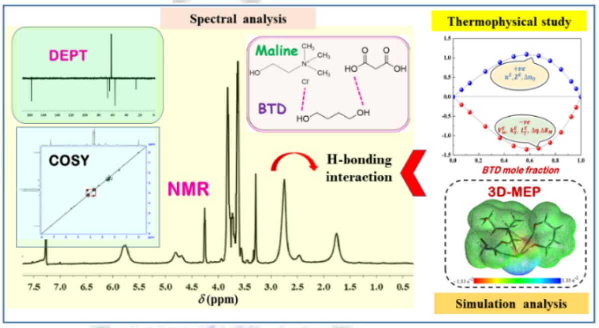
Deep eutectic solvent (DES) is emerging as a new class of eco-friendly and a cost-effective solvent. In this study we elucidate the spectral, simulation and thermophysical properties of prepared DES named as *Maline* (equimolar mixture of Choline chloride (ChCl) and Malonic acid (MA)) in the presence of an additive: 1, 4- butanediol (BTD) as *cosolvent*. Detailed scrutiny of favorable molecular networks *i.e.*, hydrogen bonding in *Maline* in the presence of BTD is investigated employing multivariate spectral techniques. The spectral results are further supported by theoretical simulation. Furthermore, to emphasize the presence of favorable interactions within the examined binary system, various thermophysical properties calculated *viz.*, the excess molar volume, V_m^E, excess isentropic compressibility, κ_S^E, excess intermolecular free length, L_f^E, excess speed of sound, u^E, excess acoustic impedance, Z^E, and deviation in viscosity, $\Delta\eta$, deviation in refractive index, Δn_D and deviation in molar refraction, ΔR_M. The excess and partial molar volumes at infinite dilution also calculated. Thus, combining the above studies will root the DES as an independent and highly advantageous *green* solvent for various organic transformations.



Schematic anticipation of molecular interaction from the properties (spectral, simulation and thermophysical study) of maline as DES and its binary mixture with 1,4-butanediol.

Keywords: Deep eutectic solvent (DES); Hydrogen bonding; Spectroscopy; Computational simulation; Thermophysical study

OP-61

Structural and dielectric properties of magnesium spinel ferrites synthesized in presence of solanum lycopersicum extract

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Spinel ferrite is the most extensively used family of ferrite. High values of electrical resistivity and low eddy current losses make them ideal for their use at microwave frequencies to control transmission path, frequency, amplitude and phase of microwave signals, surface mount devices (SMD) and multilayer chip-inductors (MLCI). A considerable attention has been paid to the synthesis of magnesium ferrite ($MgFe_2O_4$) due to its precisely controlled size and tailored magnetic properties which play an important role in cancer treatment using magnetic hyperthermia. Nowadays, the use of a low cost, environment friendly domain, waste reducing and renewable sources for energy storage is appeared to be important to reduce or eliminate the use or the generation of hazardous substances in the design, manufacture and application of chemical products. The tomato (Scientific name: *Solanum lycopersicum*) is a fruit of short lived perennial plant in the Solanaceae family. In the present study, Magnesium ferrites ($MgFe_2O_4$) were synthesized with and without presence of *Solanum lycopersicum* by sol-gel auto combustion method. In present study $MgFe_2O_4$ ferrite precursors were prepared in presence of *Solanum lycopersicum* extract heated at 650 °C, 750 °C, 850 °C, 950 °C and 1050 °C for 4 hrs. All heated samples were characterized by XRD, FTIR and dielectric measurements in order to investigate structural and dielectric properties. XRD analysis of all samples synthesized using Solanum lycopersicum extracts shows pure phase. FTIR analysis shows the absorption bands between 510-460 cm^{-1} in all the samples which are attributed to stretching of Fe^{3+}-O^{2-} vibrations. Dielectric measurements of all samples were recorded at room temperature between the range of 10 Hz to 2 MHz. It was observed that all samples show frequency dependent phenomena.

OP-62

Greener synthetic access to acridines and acridinium ions and their application in photocatalytic organic transformations

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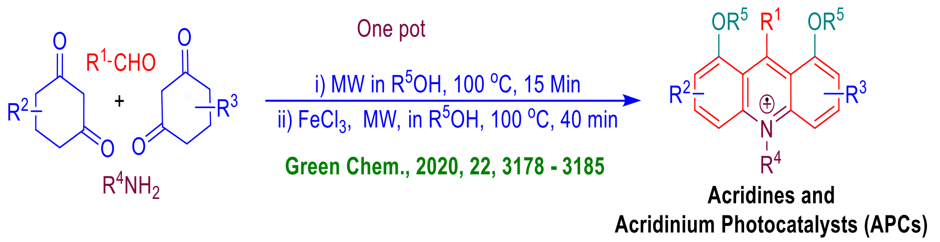
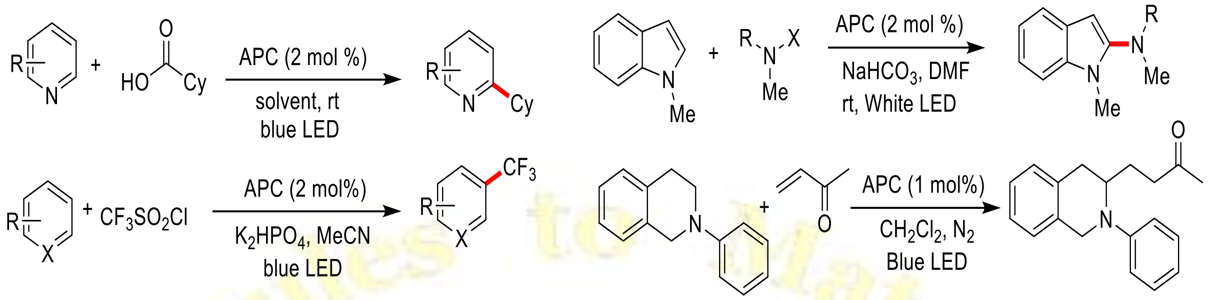
Acridines and Acridinium ions are one of the earliest known important classes of hetero-aromatic compounds with broad research and industrial applications in the field of medicinal chemistry, dye, chemosensor, photo catalysis, solar cell and photovoltaic applications.[1,2] All the synthetic methods reported for their synthesis so far mainly deal with construction of a new 6-membered ring through formation of any one or two bonds on suitably substituted pre-existing aromatic system.[3] In most cases, these aromatic precursors are not commercially available, often difficult to prepare, require multiple steps, often involve application of toxic heavy metals and ligands. We have developed a $FeCl_3$-alcohol catalyzed stepwise and one-pot general synthetic method for both diversely substituted acridines and acridinium ions directly from easily available 1,3-diketones, amines and aldehydes using molecular oxygen as terminal oxidant to produce water as the only by-product.[4] This ligand free approach has exploits high atom economy and diversity of multi-component reaction (MCR) to merge with a novel $FeCl_3$ catalyzed oxidative dehydrogenation to be the first synthesis of acridine and acridinium ions from aliphatic precursors and hence provides an effective greener alternative to all reported synthetic procedures so far. The newly generated acridinium photo-catalysts generated from this methodology found to be very effective in carrying out many vital organic transformations with exceptional ease in minimal catalyst loading without requiring any expensive heavy metal complex photocatalyst. In this presentation I shall discuss about the advancement achieved in synthesis of acridinium based photo-catalysts and effectiveness of these catalysts for providing greener alternative to several vital organic transformations.

Key words: Green synthesis, Acridines, Acridinium ions, catalysis





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OP-63

Synthesis and Characterizations of Zeolitic Imidazolate Framework – 8 (ZIF-8) and ZIF-8/PVDF Membrane for Pervaporative Separation of Aqueous Mixture

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The recent trend explored the viability and applicability of nanostructure's metal-organic frameworks (MOFs) for a new type of nanocomposite membrane synthesis. Zeolitic Imidazolate Framework-8 was found to have a well-defined pore structure, high regularity, and excellent thermal and chemical stability. In this study, we fabricated a new hybrid mixed matrix membrane (ZIF-8/PVDF) by immobilizing ZIF-8 particles onto the surface of the polyvinylidene fluoride (PVDF) membrane. The ZIF-8 crystals were prepared by the direct crystallization method. The synthesized particles and membranes were characterized by X-ray diffraction (XRD), Scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDX), Fourier transform infrared spectroscopy (FTIR), and Thermogravimetry analysis (TGA). The water contact angle analysis studied the effect of the ZIF-8 on membrane hydrophilicity.

Keywords: Metal-Organic Frameworks (MOFs), Zeolitic Imidazolate Framework-8, ZIF-8/ PVDF membrane, Characterizations

OP-64

Citric acid/ Glycerol ester, a backup of 2, 2-Bis(hydroxymethyl) propionic acid and biobased synthesis of anionic polyurethane dispersion

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Polyurethane dispersion is a modified version of polyurethane containing one or more hydrophilic groups in the polymer backbone. This modification was objectified to minimize the negative impacts of volatile organic solvent (VOCs) on the environment via the dispersion of the pristine polyurethane. The main applications of polyurethane dispersion include paintings, coatings, and adhesives, etc. Also, Polyurethane dispersion can revamp further to minimize the corrosion issue in wood and metallic surfaces. In this report, Polyurethane dispersions films with three different compositional ratios of GECA (glycerol ester of citric acid) and dimethylolpropionic acid (DMPA) were synthesized and analyzed their stability, physical and chemical properties. Different analytical techniques including FTIR, NMR, and GPC were performed to characterize the synthesized product. Besides, thermal and mechanical stability were obtained by using the standard methods and instruments.

Keywords: Citric acid, Glycerol, Castor oil, and polyurethane dispersion.

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OP-65

Titania supported Platinum nanoparticles for catalytical applications: Oxidation of Alcohols

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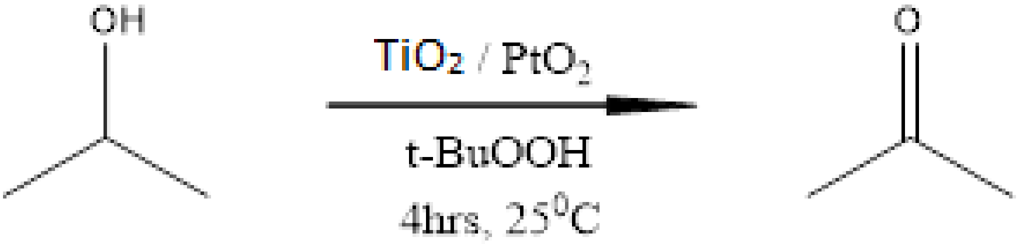
Converting the hydroxyl group into compounds containing carbonyl group (synthesis and selective oxidation of alcohols to aldehydes) is one of the challenging jobs for a synthetic organic chemist. Suitable catalysts such as metals or metal oxide nano particles, support catalysts etc. has been used either in homogenous or heterogeneous medium to carry-out this. In the process although some of catalysts being used are generated back, the reactions generate significant amount of toxic materials along with the desired products. The present work is dedicated to the rational design and development of Titania (TiO_2) supported Platinum nanoparticles for catalytical applications in the oxidation of alcohols. TiO_2 supported metal catalysts with strong metal support interaction; chemical stability has attracted interest as they have high activity for various electron transfer reactions. TiO_2 (a *n*-type semiconductors due to its wide band gap of 3.2 eV) under ultraviolet light, possess high physical and chemical stability show a high potential in photocatalyst-related applications as well.

The catalyst samples were prepared through wet impregnation of TiO_2 with PtO_2 (in 1:1 ration) in presence of dichloromethane by stirring in a magnetic stirrer for 24 hrs until a uniform paste is obtained. For characterization of the catalyst, the IR spectra were recorded using Shimadzu 8400S FTIR spectrophotometer, 2 MLH magnetic stirrers (Remi Equipment) is used for stirring, shape and size of the synthesized catalyst was investigated by SEM using ZEISS Scanning Electron Microscope. Magnetic susceptibility measurements were performed using a CTI cryogenic 8200 (Oscillator: voltage = 5 volts, frequency = 330 Hz). The oxidation states of surface components and the near surface composition of the catalyst samples were investigated using X-ray photoelectron spectroscopy, XPES (SPECS, X-ray photoelectron spectrometer).

To study the catalytic activity, alcohols (1 mmol) and the catalyst 3.5 mol% in t-BuOH were stirred at 25^{0}C for half an hour. To this t-BuOOH (2 mmol) in hexane (10 ml) was added and stirred using a magnetic stirrer for 4 hours. A typical conversion is shown in the following scheme.



Keywords: Support catalyst, Alcohol, XPES, SEM, Nanoparticle

OP-66

Physicochemical characterization and reaction condition optimization of titanosilicate-supported CoAgMn catalyst for Fischer-Tropsch synthesis

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Fischer-Tropsch synthesis is an attractive process to produce fuel-grade liquid hydrocarbons from a mixture of CO and H_2. In this work, 15 wt. % cobalt was loaded on mesoporous titanosilicate support along with promoters Mn and Ag in the atomic ratio (Co: Mn: Ag = 100:10:1) using incipient wetness impregnation. The catalysts were characterized using BET, XRD, H_2-chemisorption, TPR and XAS. The addition of promoters facilitated the reduction of the catalyst at a lower temperature (340 °C to 315 °C); however, the extent of reduction after 18 h of reduction in hydrogen at 400 °C remained constant. The Fischer-Tropsch activity of the synthesized catalyst was studied using a fixed-bed reactor after in situ reduction. The activities of the catalyst were determined by analysing the tail gas using an online GC. The CO conversion and C_5+ selectivity of the catalyst were found to be 86% and 76% respectively at reaction conditions of 220 °C, 250 psi and 2000 $mL_{syngas}/mL_{catalyst}/h$. The interaction of process parameters: temperature, pressure, and space velocity- were studied using Box-Behnken statistical design. The effects of the input variables on the CO conversion and C_5+ selectivity were statistically analysed using analysis of variance (ANOVA). The results suggested a comparatively major effect of temperature on the both the CO conversion and C_5+ selectivity. The optimum reaction conditions were determined to be 219 °C, 300 psi and 1800 $mL_{syngas}/mL_{catalyst}/h$ with a corresponding CO conversion and C_5+ selectivity of 87% and 81% respectively.

PP-01

UV Spectrophotometric Method Used For the Analysis of Torsimide in Biological Fluids and Pharmaceutical Formulations

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The simple and sensitive spectrophotometric method for the determination of Torsimide reacts with 1 ml of DDQ (2, 3 –dichloro -5, 6-dicylano-1, 4-benzoquinone) by charge –transfer complex method. In this method the drug Torsimide as n-electron donors with acceptor 2, 3 dichloro-5, 6- dicyano 1,4- benzoquinone (DDQ) to form Dark red color charge-transfer complexes. This reaction is instantaneous and quantitative. The drug maximum absorbance at 460 nm and Beer's law limit was obeyed at 25-175 µg/ml. The optical characteristics of the proposed method such as molar absorptivity, sandell's sensitivity, slope and intercept were 0.54084. $L.mole^{-1}\ cm^{-1}$, $0.0025µg.cm^{-2}$, 0.0055 and 0.0019 the correlation coefficient is 0.9999 for Torsimide respectively. The developed method was found to be simple, specific, robust, accurate and precise for the determination of Torsimide.

Keywords: Torsimide, DDQ, chloroform, methanol, UV Spectrophotometric Method.

PP-02

Vitamin B6-cofactor fluorescence dyads for the optical sensing of multiple analytes

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Cations, anions and amino acids are indispensable to life and its play vital role in biochemical functions[1, 2]. However, higher concentration and accumulation of these ions can lead to many adverse health effects. Hence a great deal of attention has been devoted to the detect metal/anions and neutral species. Several methods have been developed to analyse these ionic species but many method requires time-consuming procedure and need sophisticated instrumentations[3]. Fluorescence techniques[4] are found to be well suited to investigate the photochemical properties of the components even low cost, simple equipment and easy to handle. Herein we have reported two novel probes based on the pyrene (**1**) and dansyl conjugates (**2**) for the selective recognition of cation, anion and neutral species. The sensitivity, selectivity, binding mode and LOD of the chemosensor **1** and **2** was investigated by ATR-FTIR, UV-Vis absorbance, fluorescence spectroscopy, ^{1}H-NMR, life time and HRMS studies. After binding of metal ion, both the compounds **1** and **2** displays significant change in the emission spectra. Further the reversibility of metal complex (*in-situ*) was checked with different anions and amino acids and it shows good results. Finally the sensing system was successfully applied into the intracellular live cell imaging.

Keywords: Fluorescence sensor, Amino acid, dansyl derivative, Live cell imaging, dyads

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PP-03

A colorimetric and ratiometric fluorescent sensor for biogenic primary amines based on dicyanovinyl substituted phenanthridine conjugated probe

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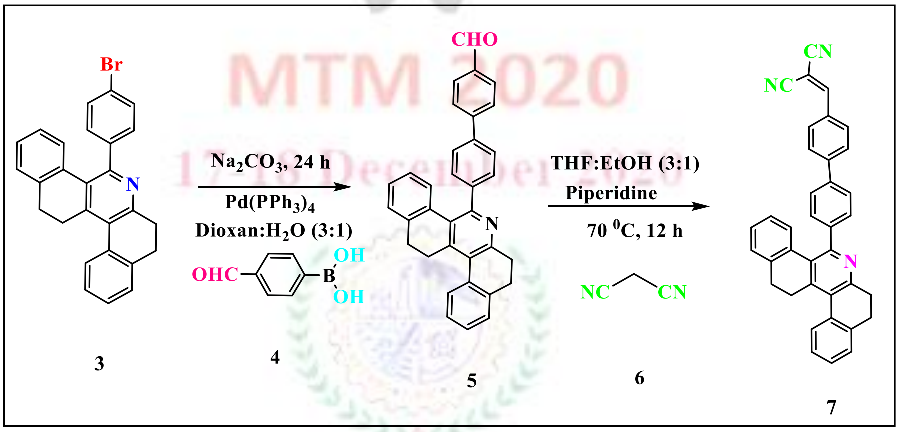
Two molecules with an aldehyde donor 4'-(7,8,13,14-tetrahydrodibenzo[a,i] phenanthridin-5-yl)-[1,1'-biphenyl]-4-carbaldehyde (**5**) and a dicyanovinyl acceptor 2-((4'-(7,8,13,14-tetrahydrodibenzo[a, i] phenanthridin-5-yl)-[1,1'-biphenyl]-4-yl) methylene) malanonitrile (**7**) were synthesized, and both were applied to remarkable solvatochromism studies. In this study, we have proposed a new method based on dicyanovinyl substituted phenanthridine moiety of **7** for selective and efficient recognition of biogenic primary amines (BPAs), based on the interaction between amine and the dicyanovinyl-linked phenanthridine moiety of **7**. It can be cleaved quickly with significant changes in fluorescence (from orange to blue) that produced **7-imine** with induced ratiometric fluorescence. UV-visible/ fluorescence spectral titration, NMR, mass spectra and DFT spectroscopic studies were proved by the mechanism of amine sensing. Limit of detections 3.67 nM (DA), 28.3 nM (EDA), 65.3 nM (HA) and 15.8 nM (n-BA) are also obtained for this probe **7** with remarkable ratiometric fluorescence enhancement. Additionally, fluorescence test paper with probe **(7)** was also fabricated and utilized to detect amines.



Key words: Phenanthridine, sensing, ICT, fluorescence, LOD

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PP-04

Switch on fluorescence sensor for selective recognition of F^- and its molecular logic gates behaviour

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Loutonin based emissive probe (L) for the dual sensing of fluoride (F^-) and bisulphate (HSO^-) anions in aqueous media. The development is based on reports that the interaction between fluoride and loutonin based fluorescent probe exhibits rapid and remarkable color changes in both colorimetrically as well as fluorimetrically. More amusingly, on the introduction of bisulphate ion into the medium containing loutonin fluoride ion complex ($L\text{-}F^-$) which shows both the color and fluorescence has been recovered. The limit of detection for fluoride ions by the probe was determined as 8.62×10^{-7} M by fluorescence titrations. Further the probe L can be employed for the removal of fluoride ions. The need for a dual anion detection system with such an outstanding reversible and reproducible process characteristics led us to consider loutonin as a feasible nominee for the construction of molecular keypad lock and molecular logic circuits. The fluorescence change of loutonin after appendage of fluoride ions is mainly due to the hydrogen bonding interaction. Further, the probe could be potentially incorporated into the test strips and silica gel plates, with better selectivity for fluoride and bisulphate anions in aqueous media.

Keywords: Loutonin, probe, Molecular logic gates, Molecular keypad lock

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PP-05

Pt(II) based anticancer agents with (N, N) bidentate σ-donor and π-acceptor ligands: their synthesis, cytotoxic property and DNA binding

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Cis-platin was recognized as chemotherapeutic agent[1] in 1978 by FDA. Despite of its great success it exhibited severe side effects [2] such as neurotoxicity, nephrotoxicity, ototoxicity. Next generation anticancer drugs like carboplatin, oxaliplatin, nedaplatin were synthesized and recognized, which are also not fully devoid of toxicity and their effectiveness is limited to only specific types of cancer. Nowadays, researchers were keenly interested to find out a safer and more effective drug. Thiols or thio-ethers of protein and peptides available in our physiological system, initially form kinetically controlled sulfur-Pt adduct which further reacts with DNA to form thermodynamically controlled adduct. To explore the anticancer activity of Pt(II) complexes, herein we report the synthesis and bio-activity of cis-Pt(MAMP)Cl_2, where, MAMP = 2-[(Methylamino) methyl]pyridine as lead molecules with a good σ-donor and π-acceptor carrier ligand[3]. Based on the kinetic investigation an outer sphere associative mechanism is proposed and activation parameters ($\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$) were calculated using Eyring equation. DNA binding activity was observed by Gel Electrophoresis experiment and binding property along with their binding constants was explored by UV-Vis spectra, competitive binding experiment respectively and the result was supported by molecular docking studies. MTT assay and ROS (reactive oxygen species) generation activity of the complexes shows comparable cancer cell growth inhibition on different cancer cell lines (HeLa and HepG2) as well as minimum adverse effect on normal cell lines (L6 myotubes, HEK 293).

Keywords: Pt(II) complexes, DNA binding, Cytotoxicity

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PP-06

Thiourea based Schiff Base as a SelectiveColorimetric and Fluorescent Chemosensor for Hg^{2+} ion with “Turn-Off” Fluorescence Responses

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An efficient thiocarbohydrazide based fluorescence sensor **STPA** for the selective detection of Hg^{2+} in semi-aqueous medium has been successfully designed and synthesized. The absorption (UV-Vis) and emission (fluorescence) properties of **STPA** were studied in various solvents. The sensor **STPA** displayed no distinct changes in absorption with various solvents; however some remarkable changes were noticed in fluorescence studies. Solvent dependent spectral characterization of **STPA** was explored via the Lippert-Mataga plot. UV-Vis and fluorescence studies also revealed that the sensor **STPA** could selectively detect Hg^{2+}ion over the other tested metal ions. The interaction of **STPA** withHg^{2+} leads to colour change from colourless to yellow. The observed quenching in fluorescence intensity may be due to chelation enhanced fluorescence quenching (CHEQ). The sensing mechanism was arrived through DFT and ^{1}H-NMRtitration studies. The limit of detection was found to be1.26 nM with a wide pH range of 4–10. Moreover, sensor **STPA** could demonstrate sensing efficiency for lower concentrations of Hg^{2+} in real sample analysis. Its performance, as a test strip and in analysis of various water samples conferred its superior selectivity.

PP-07

Synthesis, characterisation and theoretical studies of a series of Iridium (III) heterolepticcomplexes with Schiff base ligands

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Iridium (III) heteroleptic complexes with phenyl pyridine (ppy) back bone are designed to produce luminescent complexes. Typical complex incorporating two phenyl pyridines and one ancillary ligands is a common synthetic strategy for variety of mononuclear Ir(III) complexes with varied luminescence properties in solution and solid states. The phenyl pyridine ligands provide the right separation of HOMO-LUMO energy levels to radiative decay of excited electron of MLCT origin. We have designed and synthesised a series of Iridium (III) complexes with two ppy ligands along with three different Schiff bases. The crystal structures confirm the inclusion of two phenyl pyridines and one Schiff base ligand around the Ir(III) centre. Contrary to the expectation it was found that all the new complexes are non-luminescent. We looked for the reasons for such non-emissive properties. Combined with experimental observations, theoretical calculations were carried out to explore the exact causes. The calculations give the composition of HOMO and LUMO orbitals and predicted the absorption spectra in dichloromethane medium. The comparison of calculated absorption λ_{max} values with spectral data obtained experimentally reveals that the absorptions in the visible regions originate to the ligand centred transition rather than one expected of mental centred. The HOMO-LUMO transitions are either not observed or was very weak in all these complexes. The other bands in visible region were of higher energy than normal HOMO-LUMO transitions. They were from inner HOMO orbitals to LUMO or LUMO+1 levels. The HOMO and LUMO orbital pictures also reveals the dominance of ligand contribution over metal. Thus the visible region absorption bands dominated by the intra ligand and inter ligand transitions over the MLCT bands. The relaxation of metal to ligand charge transfer (MLCT) transitions is source of metal centred luminescence. In present complexes the MLCT bands were too weak to produce any detectable emission.

Keywords: Ir(III) complex, HOMO-LUMO, luminescence.

PP-08

Synthesis and characterization of Pt(II) complexes with σ-donor ligand; their bioactivity, DNA and BSA binding and theoretical study

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Cisplatin first recognized as an anticancer drug[1] and approved by FDA in 1978 though it is not fully devoid of toxicity. To reduce the toxicity, few Pt(II) based anticancer drugs developed with proper choice of carrier ligand and labile groups. Herein, we report the synthesis and bio-activity of complexes like $[Pt(DMEEDA)Cl_2]$, $[Pt(DMEEDA)(OH_2)_2]^{2+}$ $[Pt(DMEEDA)(L\text{-}cys)](ClO_4)$ and $[Pt(DMEEDA)(N\text{-}ac\text{-}L\text{-}cys)]$for drug modelling (where, DMEEDA = N,N-Dimethyl-N'-ethylethylenediamine) [2]. Rate constants and thermodynamic parameters have been calculated and two-step associative mechanism was proposed. DNA binding activities were emphasized by different techniques as absorption and fluorescence spectroscopy, Gel electrophoresis. The concerned complexes show excellent binding affinity towards DNA (binding constants ~10^4) which encouraged us to investigate in detail of their bioactivity. Growth inhibition potential of the complexes has been remarkably higher in the hepatocarcinoma cell line (HepG2) in a dose- and duration-dependent manner, as compared to cisplatin, indicating that synthesized compounds were potent enough to trigger good to moderate growth inhibition in HepG2 along with minimal toxicity to mouse primary hepatocytes in vitro. Theoretical modelling of biotransformation from Pt-S adduct to Pt(II)-DNA adduct and DFT study like structural optimization and NBO analysis were done to assist the entire work. TD-DFT study has been undertaken to generate the simulated spectra of UV-Vis and IR to compare with the experimental spectral observations.

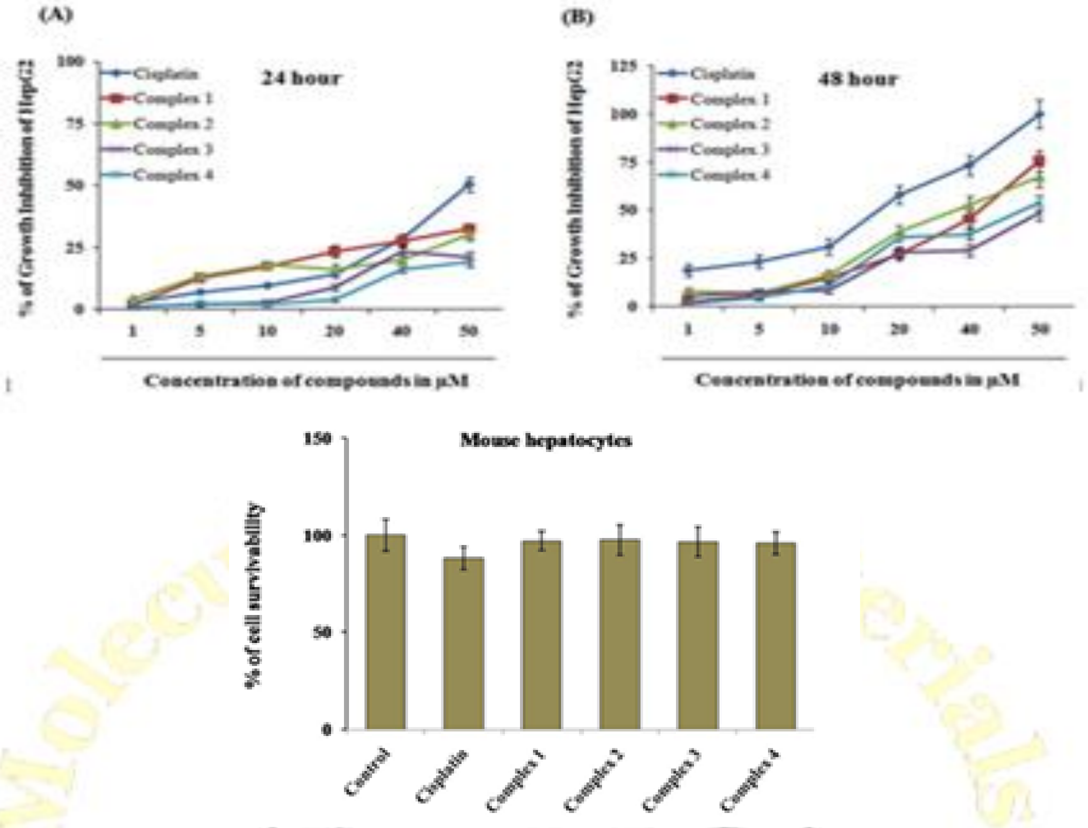

Fig.1: Cancer cell and normal cell viability in presence of Pt(II) complexes.

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PP-09

Ultrasonic Velocity and Allied Acoustical Parameters of 2, 4-dinitrophenyl hydrazine based Schiff base in DMSO

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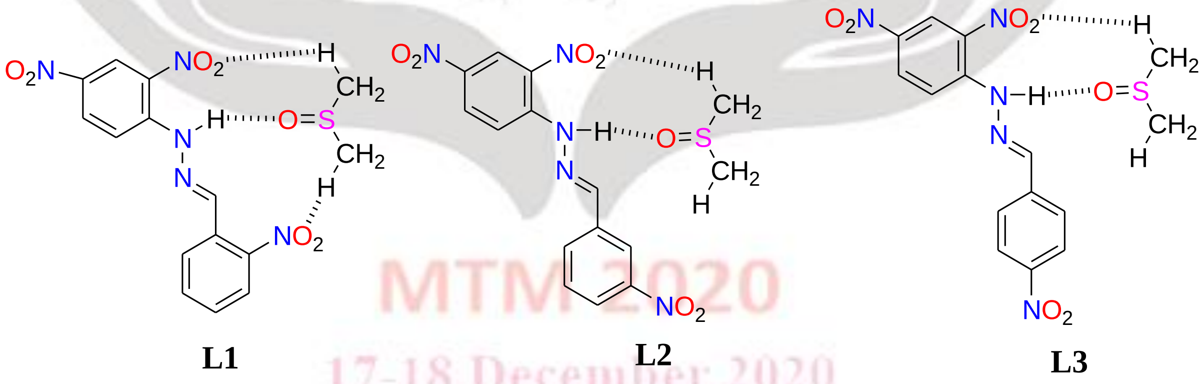
Novel 2, 4-dinitrophenyl hydrazine based Schiff bases (**L1-L3**) has been successfully synthesized and characterized. The ultrasonic velocity (C) and density (ρ) has been measured for the synthesized Schiff bases with DMSO (Dimethyl sulfoxide) solvents at 300 K. Using these experimental data ultrasonic Velocity (C), adiabatic compressibility (β_s), intermolecular free length (L_f) and specific acoustic impedance (Z) have been evaluated. From the experimental data, it has been found that **L1** ascribed higher ultrasonic velocity as compared to other molecular probes **L2** and **L3**. The strength and nature of interaction between the molecular probes and DMSO solvents has been discussed. Scanning Electron Microscope (SEM) studies of molecular probes are performed to the microstructure and surface functionalities.



Scheme 1: Plausible interactions between **L** and DMSO.

Keywords: Acoustical Parameters, Schiff base, SEM

PP-10

Synthesis and characterisation of the cis-platin analogous complex: Kinetic aspect, DFT study, DNA binding property and anti-cancer property

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Cis-platin [1,2] analogous complex [Pt(ambim)Cl_2] C-1 was synthesised with carrier ligand using 2-Aminomethylbenzimidazole (ambim). The diaqua complex $[Pt(ambim)(OH_2)_2]^{2+}$ C-2 was obtained after hydrolysis with $AgClO_4$ solution. Pharmacokinetics of C-2 with S-containing bio-molecules was investigated to explore 'drug reservoir' mechanism. DL-penicillamine (DL-pen) and Glutathione (GSH) were chosen as model bio-molecules for pharmacokinetics and synthesis of substituted complex [Pt(ambim)(DL-pen)] C-3 and [Pt(ambim)(GSH)] C-4. The kinetic studies of above-mentioned bio-molecules at pH 4.0 suggest a two-step reaction and the low value of enthalpy of activation ($H^{\ddagger}$) and negative entropy of activation ($S^{\ddagger}$) suggest an associative path. Job's method of continuous variation suggests 1:1 metal-ligand ratio in the substituted complex. DFT based calculation were performed to get an insight about the electronic structure of the complexes. HOMO-LUMO energy and for nature of electronic transition in TD-DFT were carried out as theoretical study. DNA binding property was investigated by UV- Vis titration method, EtBr displacement assay was performed by fluorescence method, gel electrophoresis and molecular docking studies were also under investigation. Antiproliferative properties of C-1 - C-4 were probed in vitro against human cervical cancer, non-small cell lung carcinoma and hepatocellular liver carcinoma cell lines and C-2 was found to be most effective in growth inhibition in all the cell lines.

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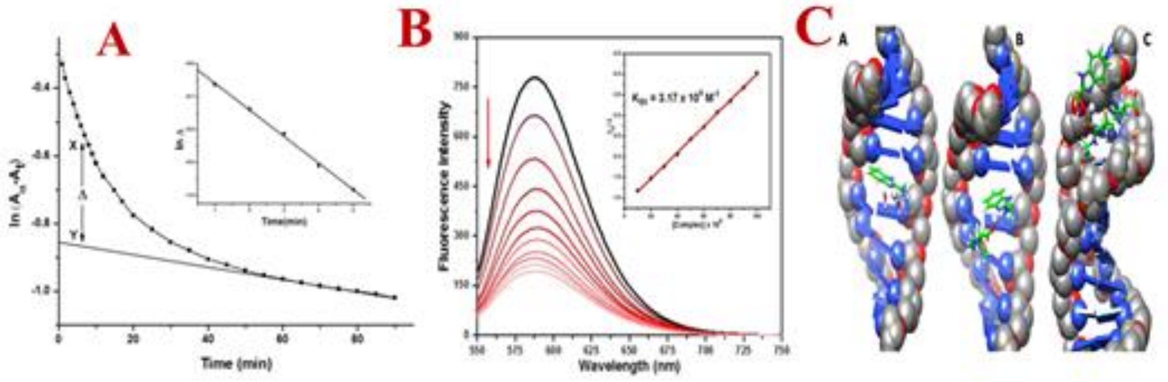

Fig.: (A) A typical plot of ln(A_α– A_t) vs time., (B) Fluorescence spectrum and (C) Molecular Docking

PP-11

Ionic liquid mediated esterification of agarose – A new sustainable method for functionalization of seaweed polysaccharides

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A new sustainable method for functionalization of agarose, a red seaweed polysaccharide using recyclable ionic liquid (IL) medium is demonstrated. The seaweed polysaccharide is esterified with succinic anhydride (SA), phthalic anhydride (PA) and maleic anhydride (MA) using 1-butyl-3-methylimidazolium bromide ([Bmim]Br) as solvent for the reaction. Half ester formation of the agarose polysaccharide was confirmed by NMR and FT-IR studies.

Keywords: Seaweed polysaccharide, Agarose, Ionic liquid, Esterification

PP-12

Synthesis, Characterization, Biological studies of Metal (II) Complexes of Nicotinamide

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A new novel Mannich base Ligand from nicotinamide derivative and its metal complexes with Cu(II) and Zn(II) ions have been synthesized and characterized. Their structural features have been established on the basis of analytical, magnetic, conductance, FT-IR, UV-visible and NMR spectra of synthesized compounds were recorded and discussed. On the basis of color, magnetic moments and electronic spectral data, the square planner geometries of Cu(II) and Zn(II) complexes have been assigned. The antimicrobial activity of the ligand, Cu(II) and Zn(II) complexes have been studied with the microorganisms such as *Escherchia coli, Staphylococcus aureus, Aspergillus niger* and *Candida albicans*, employing agar-well diffusion method. The antimicrobial studies show that the Cu(II) complex is good active than ligand and Zn(II) complex.

Keywords: Mannich base; metal complexes; geometry; redox behavior; antimicrobial activity: Antioxidant

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PP-13

Self-assembled Polymersomes loaded with CuNPs: A smart nanoreactor enabling C-N coupling via Cascade synthesis in water

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Polymersomes with various morphologies have been known to serve as nanoreactors for organic transformations. The amphiphilic copolymers self assemble non-covalently into polymerosome (i.e, polymer vesicles) and exhibit unique morphology with hydrophobic membrane and hydrophilic core. Such polymeric vesicles not only protect the catalyst within its compartment, but also facilitate a facile on-site isolation of reactive compounds enabling cascade reactions. They possess the ability to convert hydrophobic substrates in water and also facilitate facile catalyst recovery. Over the past few years researchers have reported several surfactant based nanoassemblies such as micelles, vesicles, and microemulsions functioning as nanoreactors. However polymer derived nanoreactors has not been investigated. The preliminary studies suggest that polymer vesicles function more efficiently as nanoreactors due to its stability, robustness and potential of advanced chemical functionalization for application in catalysis.

With this rational, we have developed a Cu nanoparticle loaded, surfactant free metallovesicle (CuNPs@vesicles) to function as nanoreactors for synthesis of benzimidazoles via cascade reactions in water. This work presents a unique strategy of employing environmental contaminants like nitroaniline as precursors and converting them into fine chemicals of commercial significance. It is noteworthy that the catalyst exhibits high structural integrity and stability under multiple reaction cycles.

Keywords: Polymerosome, Metallovesicle, Self-assembly, Cascade reaction.

PP-14

Synthesis, Characterization and Thermotropic Properties of Terminal Substituted Nonlinear Azoester Moiety

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A novel azo ester homologous series of liquid crystals (LCs) 2(4’ -n-alkoxy benzoyloxy) napthyl 1 azo-3”nitrobenzenes consists of eleven members of a series with enantiotropic nematogenic mesophase formation and without exhibition of smectogenic property by all the eleven homologs. The nematogenic mesophase textures are threaded or Schlieren. Solid-nematic and nematic-isotropic transition curves of the phase diagram behave in normal manner except for the decyloxy, dodecyloxy, and tetradecyloxy homologs. Analytical and spectral data confirm the molecular structures of homologues. Thermal stability for the nematic phase is 132.6 °C, and the degree of mesomorphism varies between 34 °C and 79 °C and the series if of a middle-ordered melting type. An odd-even effect is observed for the N-I transition curve with alternation of transition temperatures. The LC behavior of the series is compared with other structurally similar known homologous series to establish the relation between mesomorphism and molecular structure.

PP-15

Animal Biopolymer-Plant Biomass Composites: Synergism and Improved Sorption Efficiency

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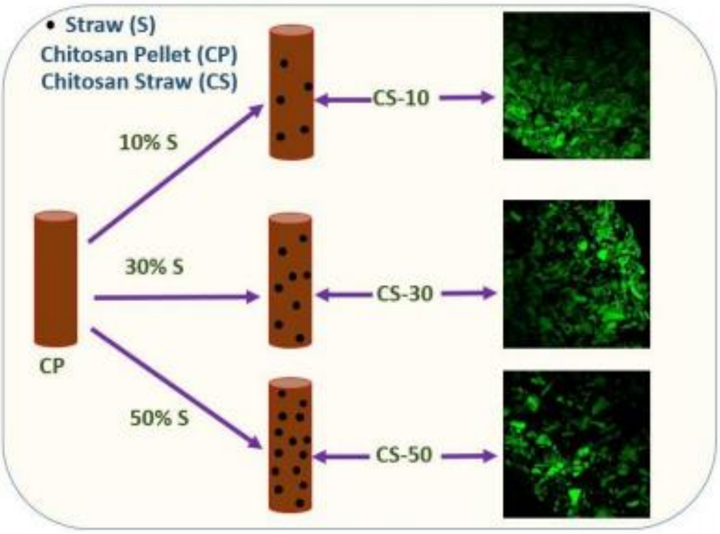
Pelletized biomaterial composites that contain chitosan (C) and torrefied wheat straw (S) at variable weight composition (C: S) were prepared using a facile blending process. The fractional content of the wheat straw was studied to elucidate the role of biomass on the pelletized product and effects of S-content on the physicochemical properties relevant to adsorption phenomena. Characterization of the chitosan pellets (with and without S) by spectroscopic (FT-IR and ^{13}C NMR) and thermal (TGA and DSC) techniques provide support for the variable C: S composition in the pellets. Confocal microscopy using fluorescein (FL) as a dye probe revealed increasing accessibility of the chitosan sites in the composite pellets that was dependent on the S-content (wt %). Equilibrium and kinetic sorption studies using FL and reactive black (RB) dyes revealed an incremental adsorption affinity of the pellets with anionic dyes in variable charge states (FL and RB). The trend for dye adsorption parallels the incremental S-content (wt %) in the composite pellets. The pelletized materials reported herein display great potentials for use as sustainable adsorbents for the sequestration a wide range of anionic contaminants from wastewaters. This study reports a first-example of a low-cost, facile, and sustainable approach for the valorization of straw and chitosan suitable for sorption-based applications in aqueous media.



PP-16

Insilico evaluation of Combinatorial and synergistic effect of Glucose transporter inhibitors and Monoclonal Antibodies associated with cancer

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Cancer is a condition of the uncontrollable proliferation of cells. In the Hypoxic conditions of cancer, GLUT protein expression increased due to more carbohydrates requirement in its metabolism. Commercially available Humanized Monoclonal antibodies like CETUXIMAB, RITUXIMAB, and ALMETZUMAB are used to treat several kinds of cancers. Recently, several kinds of GLUT Inhibitors like BAY876, Facentin, WZB117, and STF-31 that targets GLUT proteins, used in cancer therapy. As there are 14 different types of GLUTs are there, GLUT Inhibitors are suggested to use only against one or two GLUT proteins for which, we performed modeling and protein structure validation for all the fourteen GLUT proteins. These modeled proteins were docked with GLUT Inhibitors by AUTODOCK VINA and suggested the best GLUT-GLUT Inhibitor combination. Docking studies performed for Monoclonal antibodies with their receptors. In this paper, the best GLUT inhibitor among the four for every GLUT protein was identified for all the fourteen GLUTs by molecular docking. The Protein-Ligand interactions between GLUTs & GLUT Inhibitors and Protein-Protein interactions between Monoclonal antibodies and their receptors were analyzed. Based on the docking energy values and types of interactions between the molecules, several combinations of GLUT Inhibitors with Monoclonal antibodies calculated virtually. Several best GLUT Inhibitor & GLUT combinations suggested to give along with Antibody therapy to treat different types of cancers based on the Molecular docking.

Keywords: Cancer, GLUTs, GLUT Inhibitors, Monoclonal Antibodies, Docking.

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PP-17

Development of Ruthenium (II)-para-Cymene Complexes of Aryl substituted Imidazo-1, 10-Phenanthroline as Anticancer Agents

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Ruthenium complexes are currently significant attention in medicinal chemistry as they offer various properties which make them an appropriate choice for drug development. Herein, a series of ruthenium (II)-p-cymene-2-aryl-imidazo-1, 10-phenanthroline derivatives (**4a-4j**) have been prepared and characterized by various spectroscopic techniques. The structural and chemical properties reveals that Ru(II) complexes have got rigidity, planarity, aromaticity, hydrogen donating and accepting capability which tune solubility in aqueous medium and interaction with biomolecules. The association constant of these complexes with DNA and BSA were found to be 10^4–10^6 M^{-1}. The competitive displacement of ethidium bromide (EtBr) from DNA in the presence of complex reveals an intercalation or groove binding further this was supported by viscosity and in-silico studies. The cytotoxicity study of these Ru(II) complexes were conducted with two cancer cell lines (MDA-MB-231 and HeLa) and one human embryonic kidney cells (HEK-293). The study revealed that **4e**, **4f** and **4g** were found exhibit least inhibitory concentration (IC_{50}) and high selectivity with respect to HeLa and MDA-MB-231 cell lines.

Keywords: DNA and protein interaction, *In-vitro* cytotoxicity, *In-silico* design

PP-18

Design and Development of Polysaccharide based Biodegradable material for tailor made applications

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The present research work is a study of a method of preparation of a Biodegradable material/film. In the method, sodium alginate (SA) and Guar Gum was used as a matrix, glycerol as plasticizer, and Glutaraldehyde as a cross-linking agent. The resulting solution of the above mentioned combination was highly viscous. The film was prepared using solution casting method and dried using an oven. The method was optimized in terms of combination of polysaccharides, molar ratios of the crosslinkers and plasticizer. The optimum material/ film was selected for further characterization and to study physicho-mechanical properties. From the study, it is concluded that the film obtained haspromising mechanical properties and the film biodegradability was also not affected.

PP-19

Renewable Starch Carriers with Switchable Adsorption Properties

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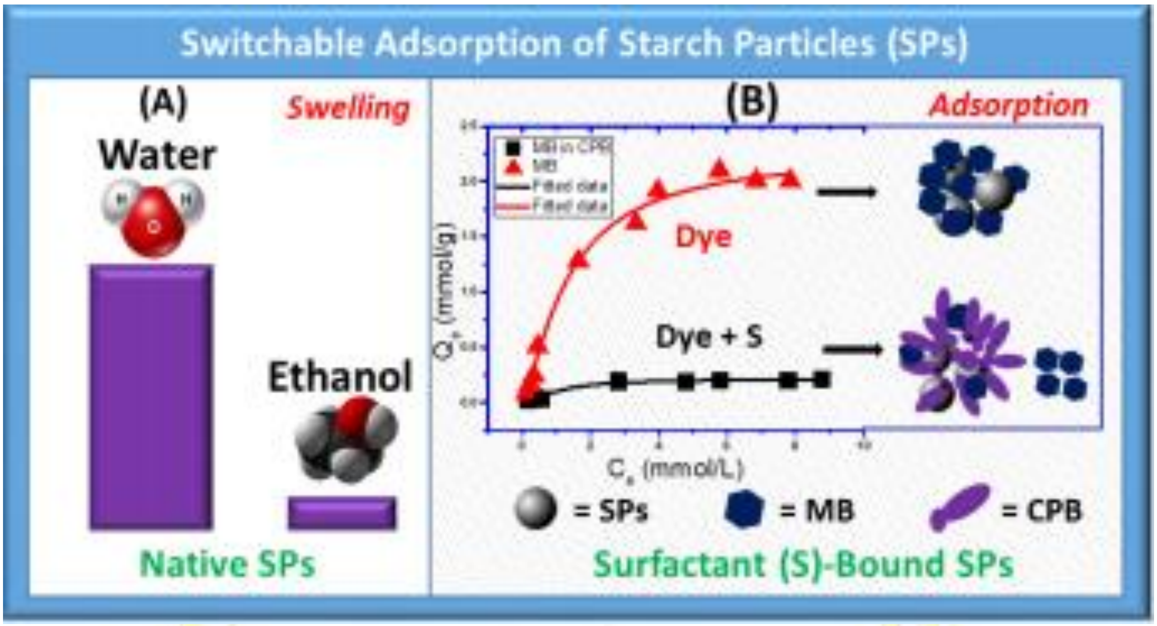
This research describes a systematic study on the structure and sorption properties of Carnation-based starch-particles (SPs). The structural characterization utilized spectroscopy (NMR, FT-IR), scanning electron microscopy (SEM), and thermal analyses (DSC, TGA). The sorption properties of the SPs were characterized by gravimetric solvent (water, ethanol) swelling and via uptake of cationic adsorbates [methylene blue (MB) dye and cetylpyridinium bromide (CPB) surfactant] at equilibrium and kinetic conditions. The surface area (SA; ~3 – 580 m^2/g) of the SPs was estimated using nitrogen gas and dye adsorption isotherm methods, where the range in SA relates to solvent swelling effects on the textural properties. The unique solvent swelling properties of the SPs reveal greater swelling in aqueous (water) over organic (ethanol) solvents. Furthermore, SPs display preferential equilibrium uptake of MB dye (Qm ≈ 716 mg/g) over CPB (Qm ≈ 292 mg/g); whereas, surface-doping of CPB onto SPs lowered the uptake of MB by an order of magnitude (Qm ≈ 67 mg/g) due to competitive binding and alteration of the surface functional properties of the doped material (Scheme 1). The doping of SPs with a surfactant (e.g. CPB) provide a facile approach for tuning of various surface functional properties; hydrophile-lipophile character, surface charge, anti-bacterial activity, and hydration properties of the SPs for targeting cationic and anionic pollutants and excipients. Evidence of monolayer and multilayer adsorption of CPB onto SPs leads to switchable adsorption properties where such amphiphile surface patterning can be harnessed to yield materials with unique controlled catch/release properties for various applications.



Scheme 1. (A) Gravimetric solvent swelling of SPs in water and ethanol. (B) Dye uptake on pristine SPs (Red) and surfactant (CPB)-doped SPs (black).

PP-20

Synthesis and Characterization of Analcime Type Zeolite Using Waste Coal Fly Ash and its Application as an Adsorbent

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Fly ash is harmful and its disposal / utilization is the major issue from environmental point of view. Generally, waste coal fly ash (CFA), generated in huge quantity in thermal power plants, and its conversion into useful materials for various applications is one of the thrust research areas in recent times. As, fly ash contains silica and alumina in its composition and thus, can be used as silica, alumina source in zeolite synthesis. Synthesis of different zeolites, mainly zeolite X, P and zeolite A types from coal fly ash are reported in the literature [1, 2]. In our continuous efforts towards the development of fly ash based zeolitic materials, previously we have developed Mordenite type zeolite using lower fly ash utilization per batch, while in the present endeavor an attempt has been made to prepare Analcime zeolite (FANA^{H}) using maximum utilization of waste coal fly ash per batch. In order to enhance fly ash utilization, the molar composition of Na_2O in the batch is also increased from 6 to 12 M, in order to get maximum dissolution of silica and aluminium from the waste coal fly ash. The materials thus synthesized shows typical characteristics peaks of Analcime zeolite. The resultant materials were characterized by XRD and SEM to identify zeolite phase and crystal morphology. Further, the material thus obtained was utilized for the removal of Pb^{2+} metal ions from aqueous solution.

Keywords: Zeolite, Waste coal fly ash, Metal ions removal, Adsorption

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PP-21

Tollens’ reagent as an adaptable reagent for C-C oxidative coupling of phenols

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Biphenols with C_2 and C_1 symmetry are reorganized as the significant structural element of many biologically active natural products and pharmaceuticals, and also wildly used in organic transformations and catalysis. Therefore, development of methods to prepare cross coupling product is still remained active area of research. [1]

On the other hand, Tollens’ test (Fig 1a) remained confined in undergraduate practical laboratory for selective oxidation of aldehydes over ketones. In this redox reaction, aldehyde gets oxidized while $[Ag(NH_3)_2]^+$ complex gets reduced to Ag^0 by forming silver mirror on the walls of test tube. We have explored oxidizing power of silver ammine complex for C-C coupling reaction of phenols to yield Bi-phenol. The reagent was found to be recyclable, reusable (Fig 1b) and energy and time efficient as compared to present C-C Coupling reactions in literature. [1] The reaction shows applicability for number of derivatives of phenols. [2,3] We could extend this reaction to cross-coupled products and interestingly by using different surface one can alter product formation, from experimental observations and results mechanical is proposed herein. Present work underlines three important aspects, (a) explore of C-C oxidative coupling reactions of phenol using silver ammine complex; (b) explore surface influenced cross coupling; (c) study recyclability and reuse of $[Ag(NH_3)_2]^+$ complex using homo-hetero phase transfer during reaction and product formation(d) Approach to symmetric synthesis.

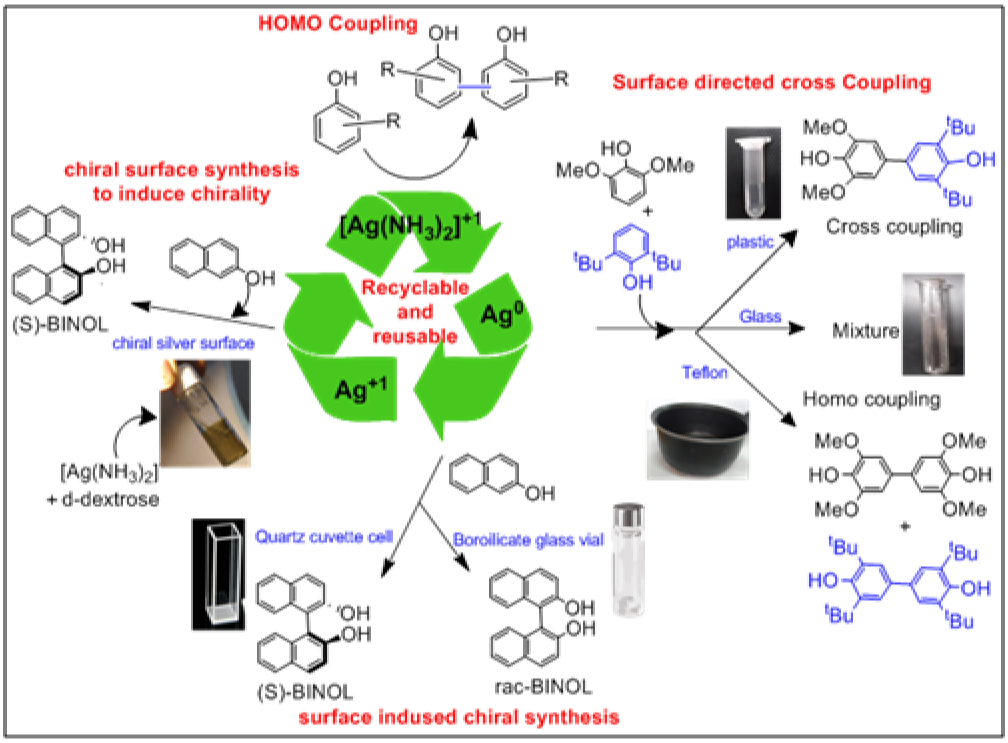

Figure 1: (A) Graph shows effect of different surface on C-C coupling of 2,6-di-tert-butylphenol (a) and 2,6-dimethoxyphenol) using using $[Ag(NH_3)_2]^+$ resulted in alter in homo-coupling product (aa and bb) and cross-coupling product (ab).

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PP-22

Upgradation of hydrothermal liquefied bio-crude via co-processing with hydro-treated heavy gas oil

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The demand for liquid transportation fuels is anticipated to remain high in the future. Therefore, to meet future demand, an avenue is provided by the utilization of non-conventional resources such as biomass-derived fuels. In the present study, we have explored the production of bio-crude using waste wheat flour and canola filtered material via the hydrothermal liquefaction (HTL) technique. Further, bio-crude blend (10% bio-oil with 90% of HHGO) was prepared and hydroprocessed (co-processing) with hydrotreated heavy gas oil (HHGO) using commercial CoMo and NiMo catalysts. Physicochemical properties (simulated distillation, moisture content, CHNS elemental analysis, ash content, GC-MS spectra, oxidation stability, thermal stability, NMR, acid value, surface properties, heating value) of the bio-crude, blend, and hydrotreated blend were determined using ASTM and AOCS standard test methods. Detailed physicochemical characterization of the bio-oil revealed that it contained 14 % of biogasoline, 56 % of biodiesel, and 27 % of waxes and asphaltenes based on boiling point distribution of the bio-crude using simulated distillation analysis, and the same was confirmed by GC-MS and NMR spectral analysis. The elemental composition of the bio-crude detected the presence of sulfur (5000 ppm), nitrogen (20100 ppm), and oxygen contents (151800 ppm), which need to be removed completely to increase the heating value and meet the liquid transportation fuel standards.

Keywords: Bio-crude, Co-processing, Hydrothermal liquefaction, Hydrotreatment, Upgradation.

PP-23

Ferrite Composite Based Microwave Absorber

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Electromagnetic pollution has turned into a deliberate affair due to the enormous implementation of high tech wireless technologies. The aforementioned situation has provoked the researchers to work in the microwave absorption domain. The requirement of a novel, unique and remarkable microwave absorbing material (MAM) is the foremost need of today's scenario. The MAM should possess qualities like good absorption, wider bandwidth, lightweight, and low cost. In this retrospect, the present paper will discuss the working principle of a ferrite based microwave absorber, a list of preferable synthesis methods, how the ferrites are chosen based on hysteresis graphs, and will conclusively state how absorption is calculated based on reflection loss calculation.

PP-24

Effect of Gallium substitution on structural and dielectric properties of X-type strontium cobalt hexagonal ferrites

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X-type hexagonal ferrites with substitution of gallium have been synthesized by using sol-gel auto-combustion method. A series of samples of $Sr_2Co_2Ga_xFe_{28-x}O_{46}$ (x= 0.0, 0.4, 0.8, 1.2, 1.6 and 2.0) were prepared in the laboratory and sintered at 1250 °C for 5 hours and then slowly cooled to room temperature. The resultant material was characterized using XRD, FTIR for its structural properties. XRD analysis show formation of X-type phase for the samples with x=0.0, 0.4 and 0.8 while W phase is dominant in the samples x = 1.2, 1.6 and 2.0. FTIR analysis reveals formation of metal-oxygen bonds in all the samples. Dielectric behavior of the prepared material under the effect of low frequency shows that substitution of gallium increases the dielectric constant to a great extent and there is enhancement in the ac conductivity for the sample with highest gallium concentration.

Keywords: X-type Sr-Co hexaferrites, Gallium substitution, FTIR, XRD, Dielectric measurements

PP-25

Solubilization of pollutant hydrocarbons in EO-PO type block copolymer micelles.

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The removal of hydrophobic pollutant hydrocarbons from aqueous medium is a challenge for today's scientists. Amphiphilic block-copolymers with an appropriate balance between the hydrophobic and hydrophilic blocks can be adopted for effective removal of these pollutants. The presence of hydrophobic polypropylene oxide (PPO) and hydrophilic polyethylene oxide (PEO) blocks in their fabrication makes these copolymers amphiphilic in nature. Triblock copolymers like Pluronics® and star block copolymers like Tetronics® are commercially available and suitable for this purpose and thus have been used in the present study.

Here we report, the solubilizing behaviour of two amphiphilic EO-PO block copolymers, linear P104 and star block T1304 with similar EO/PO ratio, for some polyaromatic hydrocarbons like naphthalene, anthracene, phenanthrene and pyrene. These copolymers undergo micellization above a certain concentration and temperature called critical micelle concentration (CMC) and critical micelle temperature (CMT). These micelles are able to trap pollutants either in hydrophobic core or keep them close to core -corona region. To identify the stability of the copolymeric micelles physical and scattering techniques are utilized. Cloud point (CP), viscosity, dynamic light scattering (DLS) and small angle neutron scattering (SANS) techniques have been utilized to check the aggregation behaviour of these block copolymers in the aqueous medium. In addition, we have tried to find out an optimum composition so as to remove these pollutants from contaminated sites effectively.

PP-26

Thermal Degradation of Zinc O, O- Diethyl dithiophosphate in n-hexadecane at 190 ^{o}C is Hydrolytic in Nature

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Zinc O,O-Diethyl dithiophosphates, the many-functional molecules have been widely used as antiwear, oxidation, and anticorrosive inhibitors in engine oils for many decades but how do they perform their functions, in particular, the antiwear function is not clearly understood. It is widely believed that they act as antiwear agents by undergoing thermal degradation forming sacrificial films on metal parts. However, the exact nature of their thermal degradation remains uncertain. Exploiting P-31 NMR spectroscopy, we report herein our results on the decomposition of zinc o,o-diethyl dithiophosphate in n-hexadecane at 190 C under conditions relevant to their usage in an actual engine environment. Thus, the zinc o,o-diethyldithiophosphate under these conditions yielded five major phosphorus containing products, O,S,S-triethylthiophosphate, O,O,S-triethyltrithiophosphate, S,S,S-triethyl trithiophosphate, O,S,S-triethyl dithiophosphate, and O,O,S-triethylthiophosphate. These products were respectively formed in 19.8, 44.9, 10.8, 4.5, and 9.3 % yields. Hydrogen sulfide was identified as a volatile product. A white solid was also obtained that gave off hydrogen sulfide upon treatment with dil. HCl indicating its zinc sulfide nature. The nature of this phosphorus containing products implicits the occurrence of thiono-thiolo isomerization coupled with disproportionation. We further discovered that the thermal degradation was hydrolytic in nature. Although we could not observe the intermedicy of o,o-diethyl dithiophosphoric acid in the thermal degradation of the zinc o,o-diethyl dithiophosphate, we discovered in independent experiments that this intermediate product arising as a result of the hydrolysis of the parent dithiophosphate, underwent the thermal degradation to give exactly the same phosphorus containing products in the same ratio as the parent zinc o, o-diethyl dithiophosphate under the same reaction conditions i.e in n-hexadecane and at 190 ^{o}C.

PP-27

An expedient in to the phase behaviour and scattering profile in PEO-PPO-PEO block copolymer mixed systems in aqueous solution

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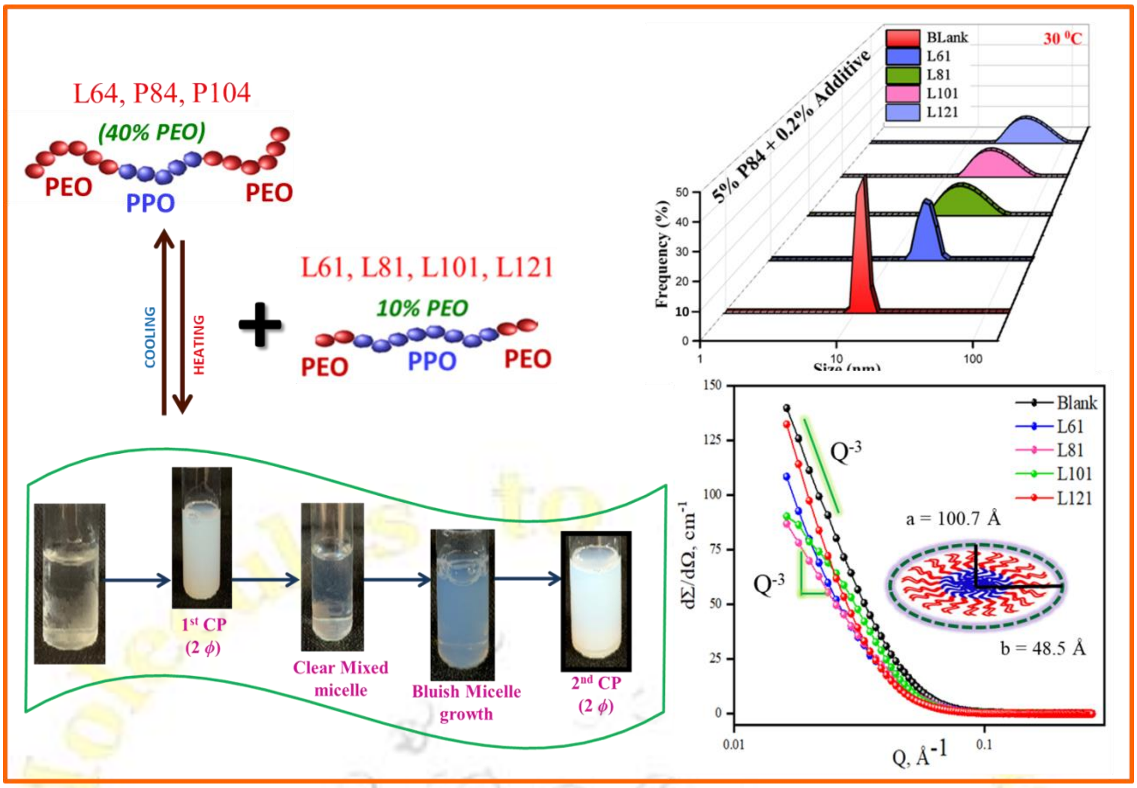
The present study aims to develop copolymeric micelles giving an account on the clouding behavior of two series of poly(ethylene oxide)-*block*-poly(propylene oxide)-*block*-poly(ethylene oxide) (PEO-PPO-PEO) block copolymers with varying molecular weight of PPO: one with moderate hydrophilicity *i.e.*, 40 % PEO (L64, P84, P104) blended with very hydrophobic copolymers *i.e.*, 10 % PEO (L61, L81, L101, L121). Marked changes in the solution behavior in our mixed copolymeric solution systems depicted the micellization and micelle growth/ transition along with the phase separation (2ϕ) well explained from cloud Point (CP) and solution viscosity study. The CP analysis showed the lower cloud point (LCP) and the conventional upper cloud point (UCP) *i.e.*, two marvelous CP in the aqueous mixed Pluronics® system which motivated to explore the hypothesis of *double* cloud point. Such shifting phenomenon from LCP towards UCP demonstrated an increment in dynamic light scattering (DLS) intensity resulting in the obvious increment in the micellar dimensions *i.e.*, hydrodynamic diameter (D_h) for the examined mixed copolymeric system. In addition, the small angle neutron scattering (SANS) data were fitted attractively in an absolute scale to obtain the predictable parameters such as, hard sphere radius (R_{hs}), aggregation number (N_{agg}) and micellar morphology. The structure of micelle remains basically steady *i.e.*, spherical micelles yet it changes quickly to elongated ellipsoidal with temperature ageing depicting a strong dependence on the amphiphilicity and concentration of the two BCPs in the mixed solution environment.

Keywords: Pluronics®; Cloud point (CP); solution viscosity; scattering; micellar transition.



Phase behavior depicting *double* cloud point (CP) and scattering portrayal of 5 %w/v Pluronics® solutions of moderate hydrophilicity (40 % PEO series) blended with varying amount of highly hydrophobic Pluronics® (10 % PEO series).

PP-28

Enhanced Durability of Fly Ash blended Cement Mortars Reinforced with Polycarboxylate Superplasticizer Stabilized Graphene Oxide

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The present study focuses on the utilization of superplasticizer stabilized graphene oxide (GO) as a reinforcing agent in the fly ash blended cement mortar (30 to 70 ratio of FA/OPC). An effort has been made to stabilize the GO via superplasticizer's (PCE-SP) steric effect and has further been used as a reinforcing agent in the cement-fly ash based mortars. The incorporation of 0.08% PCE-GO (by weight of blend) improved compressive and split-tensile strength of the mortars by 39.8% and 48.9% as compared to control sample at 90 days of curing, respectively. Mercury Intrusion Porosimetry studies shows that porosity of fly ash-cement mortar was reduced significantly as compared to control after 0.08% PCE-GO incorporation. Durability studies such as acid & sulfate attack were found to be better for fly ash based mortar as compared to pure OPC based mortar. Water absorption for 0.08% PCE-GO was reduced by 18.6% in comparison to control sample after 90days curing age. The control sample and 0.08% PCE-GO mortar showed a weight loss of 5.9% and 1.9% after 90 days of exposure to acid. However, the weight loss values were shown to be 2.7% and 0.9%, respectively, after an exposure period of 90 days to sulfate solution.

Keywords: Graphene Oxide, Durability, Physico-mechanical Strength, Porosity

PP-29

Influence of 200 MeV Ag^{16+} ions irradiation on Magnetic properties of $CoFe_2O_4$ Spinel ferrites

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The $CoFe_2O_4$ spinel ferrite nanoparticles were synthesized using a sol-gel auto combustion technique. Synthesized $CoFe_2O_4$ ferrite powder was irradiated with 200 MeV Ag^{16+} ions with the fluence of $1x10^{13}$ ions/cm^2. To study the influence of irradiation, Cobalt ferrite samples were characterized before and after irradiation. Structural and morphological properties were studied using various instrumental techniques like FTIR, XRD and SEM measurements. Magnetic properties were studied using VSM.

XRD shows the broadening of intense peaks of irradiated samples which reveals that the crystallite size decreases after irradiation. FTIR spectra for both; pristine as well as the irradiated samples, confirms the formation of strong ferric oxides bands. SEM images show that after irradiation, particles become homogeneous in size. VSM data shows that the saturation magnetization and coercivity decrease after irradiation.

Keywords: 200 MeV Ag^{+16} ions, XRD, VSM

PP-30

Simulations and Analysis of Peptide Structures in Lithium-Chloride Solutions

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Biological system depends on a diplomatic balance of noncovalent interactions.[1] The surface of proteins has great tendency to bind with the ions, and is influenced by the screening of the electrostatic potential of the ions in salt solutions.[2] Alkali metal ions interact with the protein surface, but that interactions may or may not last for too long. We carried out simulations of prion peptide structures to characterize the interactions between the salts and the peptide surface. The results show that the peptide forms different secondary structures with various concentrations of LiCl. We calculated the average backbone RMSD and average radius of gyration of the native conformation. The strength of specific interactions of ions with the peptide surface depends on the concentration of the salt. With the increase in the concentration of ions, however, the protein-ion interaction decreases due to competition between the ions to bind with the protein surface. The preferential binding affinity shows that the ions bind to the peptide surface more. Further, free energy landscapes[3] for these conformations are also performed.

Keywords: Prion peptide, LiCl, MD Simulation, Free Energy Landscap, Preferential Binding.

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PP-31

Adsorption of P103 nanoaggregates over graphene oxide nanosheets: role of electrostatic forces

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This work reveals the role of surface charge on adsorption ability of Pluronic 103 (P103) micelles over negatively charged surface of graphene oxide (GO) nanosheets. Cationization was induced by adding dodecyltrimethylammonium bromide (DTAB, a cationic surfactant) in P103 micelles until the point of de-micellization. Subsequent changes in aggregation parameters were investigated through dynamic light scattering (DLS) and small-angle neutron scattering (SANS) studies. A steady change in the zeta potential of P103 micelles was observed during DTAB incorporation. At high surface charge density, interaction between adjacent head groups was distorted and micelles dissociated. Structural developments during the adsorption of mixed micelles over sheet surface (mass fractal formation) were monitored in terms of changes in the scattering features of aggregates. These fractals emerged as a result of electrostatic interactions. Our observations indicate towards existence of small-sized building blocks at low DTAB concentration (≤ 4 mM). Charged micelles were adsorbed more effectively and maintained a hydration layer in the inter-sheet space. However, at higher DTAB concentration (≥ 10 mM), micelles dissociated to produce unimers and loose aggregates. At this point, sheets exhibited quick aggregation in spite of fractal formation.

Keywords: Graphene oxide; Block copolymers; Mixed micelles; Mass fractal; Aqueous dispersibility; Zeta potential

PP-32

Dispersion study of graphene oxide in various Polycarboxylate based superplasticizer

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In the cement composite the hydration, mechanical strength, and durability properties improved by incorporated graphene oxide (GO). A drastic change can be found in the performance of cement by adding a known amount of graphene oxide. For GO to manifest its superior characteristics as a nano reinforcement. The exact mechanism is not known now. In this, we explicate the dispersion of graphene oxide. The aggregation of graphene oxide could be reduced by the addition of a polycarboxylate based superplasticizer. Firstly, ultraprobe sonicator developed the data in UV spectrum and clears the distribution of graphene oxide. Several plasticizer has been used in the study of graphene oxide dispersion because a major problem is poor dispersion of graphene oxide is found. Aggregated graphene oxide initiates pores which directly increases porosity. The study of dispersion provides a well understanding of the conflicting behavior of various super-plasticizer on graphene oxide.

Key words: Graphene Oxide, Ultraprobe sonicator, Polycarboxylic, Plasticizer, Dispersion.

PP-33

Changes in aggregation properties of TPGS micelles in the presence of sodium cholate

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D-alpha-tocopheryl polyethylene glycol 1000 succinate (TPGS), a nonionic surfactant, has been tested clinically as bile salt sequestrant. This research was aimed at investigating the effect of sodium cholate (NaC, a bile salt) on aggregation properties of TPGS. Changes in TPGS aggregates during NaC incorporation were investigated by UV-visible spectroscopy, electron microscopy, dynamic light scattering (DLS) and small angle neutron scattering (SANS). In pre-micelle concentration regime ($\leq$10 mM), NaC molecules migrated into the micelle core and no interfacial events were recorded in terms of changes in the cloud point and conductivity of dispersion. As a result of hydrophobic association between NaC and TPGS tail, micelles exhibited 20-30% contraction. However, at higher concentration ($\geq$20 mM), micelle core became crowded. Subsequently, NaC molecules were driven towards shell region and swollen aggregates (200-300 nm) were formed. Movement of NaC to the shell region was confirmed from the bathochromic shift of methyl orange, encapsulated in the micelles. We reveal that hydrophobic interactions remarkably dominated under dehydrating effect of electrolytes, particularly under acidic conditions wherein NaC remains unionized. At intestinal pH, hydrophobic attraction appeared to be compensated by the electrostatic repulsion among ionized molecules; micelle dissociation occurred with 10 mM NaC. Our findings on TPGS-NaC interactions can be utilized to achieve successful bile salt sequestration.

Keywords: TPGS, nonionic micelles, bile salt, cloud point, aggregation, micelle dissociation

PP-34

Amphiphilic molecular activities of Star-block copolymer in water-DES mixture incorporated for Drug solubilization study

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Deep eutectic solvent (DES) have revealed the capacity to promote the aggregation of amphiphiles in solution. The self-assembly of amphiphilic substances in protic/aprotic, polar/non-polar solvents, ionic liquids (ILs) and deep eutectic solvents, we herein report the micellization and aggregation behavior of a star-block (4-arm) ethylene oxide (EO) - propylene oxide (PO) block copolymer: Tetronic T1304 in the presence of DES (Choline Chloride (ChCl) as Hydrogen Bond Accepter (HBA) with Levulinic acid (LA) as Hydrogen Bond Donor (HBD)) in varying molar ratios (1:1 and 1:2).Various Physicochemical techniques *viz.*.,Cloud Point (CP), Surface Tension (ST), Small angel neutron Scattering (SANS), Dynamic Light Scattering (DLS) were present for self-aggregation and size distribution of amphiphilic Tetronic T1304 in water-DES mixed system. The solubility of poorly water soluble anticancer drug, Curcumin (Cur), was also checked for T1304 micelles with DES using UV-Visible spectroscopy (UV-Vis). The presence of DES alters micellization i.e. it is favored at lower temperature and micellar characteristics and the observed behaviour is described as favored interactions that support the self-assembly in water-DES solvent mixture.

Keywords: Block Copolymer, Deep eutectic solvents (DES), Physicochemical Characterization, Self-assembly, drug solubilization.

PP-35

PVA bound electrolyte gel ribbon: Unravelling solid state impedance by equivalent circuit model analysis

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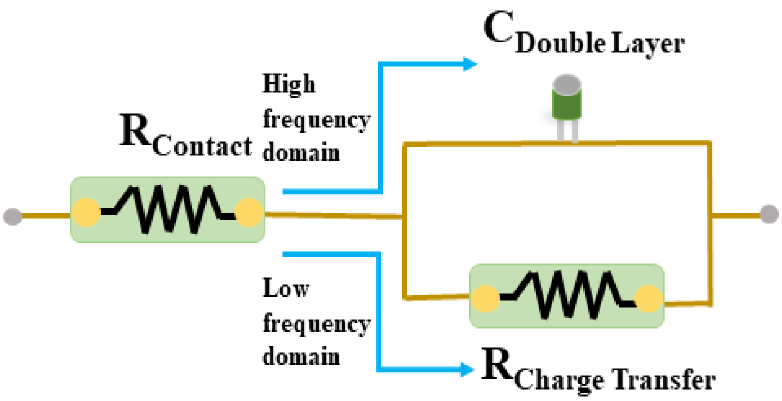
A common word we often earshot negatively in our daily life is the short circuit. Curious minds roam around, how does it happen? Where? Is it catching some fire or not? Now leaving apart the word 'short', the other picture utters immediately about the circuit is some electric model or loop where the current can flow. Essentially, our electronic realm makes a crispy vocabulary to talk about the circuit using a glossary of terms like resistor, capacitor, and inductor, etc. Indeed, an equivalent circuit refers to a theoretical circuit to retain an individual system electrical characteristic. Isn't it even more thrilling if a chemical event like a charge transfer process across a molecule with respect to time bondage can mimic an equivalent circuit model? Yes, so-called impedance spectroscopy can give us the properties of electrical components, for instance, capacitances, interfacial resistances, inductance of various devices including fuel cells, supercapacitor, organic field-effect transistors, and so on by applying sinusoidal perturbations with a broad range of frequencies. Here, we present polyvinyl alcohol (PVA) based gel electrolyte AC impedance analysis to unravel the physical processes within the vast frequency range, i.e., broad timescale using an equivalent circuit.



PP-36

Co-effect of Graphene Oxide and Carbon Nanotubes on Mechanical, Microstructural and Porosity Properties of Fly Ash based Cement Mortars

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The current study investigates the better reinforcing tendency of superplasticizer stabilized carbon nanomaterials hybrid, i.e., FCNT@GO in comparison to the individual carbon nanomaterials, i.e., either graphene oxide (GO) or functionalized carbon nanotubes (FCNTs) on the fly ash blended cement mortars (FCMs). The compressive strength for 0.08% FCNT-FCMs and 0.08% GO-FCMs (by weight percent of cement-FA blend) was improved by 24.9% and 39.8%, in comparison to Control (FA) sample, respectively, at 90 days of curing. However, for FCNT@GO hybrid incorporated mortars, a superior improvement of 52.1% was found at the dosage of 0.16%. On the contrary, the maximum split tensile strength improvement was 64.3% for 0.08% FCNT@GO-FCMs whereas, 0.08% GO-FCMs and 0.16% FCNT-FCMs showed an enhancement of 48.9% and 39.7%, respectively. These results were also compared to the Control (cement) samples. The compressive and tensile strength values for 0.16% FCNT@GO-FCMs (39.7 MPa & 5.2 MPa) were shown to be comparable or even better than the values obtained for Control (cement) mortars (37.6 MPa & 4.1 MPa). The better production of hydration products leading to the densification of the cement-FA matrix in FCNT@GO-FCMs is attributed to the synergic effect of fly ash and carbon nanomaterials in the mortar sample as examined by FE-SEM and XRD studies. Mercury Intrusion Porosimetry (MIP) showed porosity decline by 34.7%, 51.4%, and 57.8% for FCNT-FCMs, GO-FCMs and FCNT@GO-FCMs in comparison to Control (FA), respectively.

Keywords: Fly ash blended cement mortars (FCMs), Carbon nanomaterials, Microstructure, Porosity, Mechanical strength

PP-37

Structural and magnetic properties of Sm doped X-type hexaferrite $Ba_{2-x}Sm_xCo_2Cd_yFe_{28-y}O_{46}$

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A series of Samarium doped X-type barium based cobalt hexaferrite $Ba_{2-x}Sm_xCo_2Cd_yFe_{28-y}O_{46}$ ($x<0.2$, $y<0.2$) has been prepared using simple heat treatment method. The samples were heated at 1350 ˚C for 6 hrs and various characterizations like X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), and Vibrating Sample Magnetometer (VSM) have been performed on the samples. XRD analysis shows that all the samples possess the X-type phase along with minor impurities phases. FTIR analysis confirms the ferrite phase in the prepared samples. VSM analysis shows the saturation magnetization in the range of 48 to 65 Am^2/kg and coercivity under 0.01 T.

Keywords: X-type hexaferrite, heat treat method, magnetic properties

PP-38

Synthesis and characterization of processable conducting poly (m-aminophenol)

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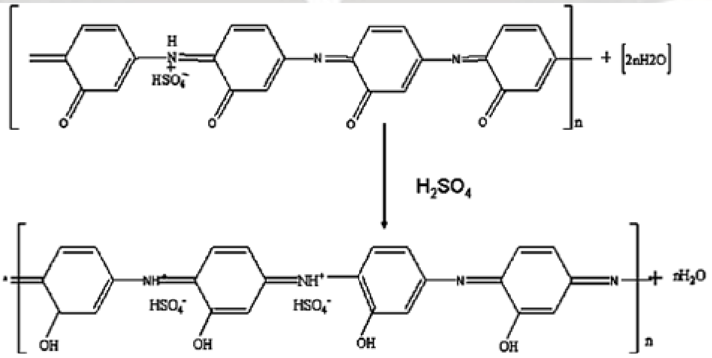
In this work, poly(*m*-aminophenol) (PmAP) was synthesized in hydrochloric acid (HCl) medium, and solubility in different organic solvents were investigated. The synthesized polymer (PmAP) was characterized by Fourier transform infrared (FTIR) and nuclear magnetic resonance (NMR) spectroscopy. It was found, the developed polymer is soluble in different organic solvents and can form a free-standing film with Dimethyl sulfoxide (DMSO). Then the polymer film was doped with both HCl and sulphuric acid (H_2SO_4) by solution doping method. The HCl doped polymer showed dc-conductivity of 8.11×10^{-8} Scm^{-1} while H_2SO_4 doped polymer showed that of 5.011×10^{-4} Scm^{-1}. From experiments and analysis, it was found that H_2SO_4 is better dopant for the synthesized polymer than HCl in terms of stability and conductivity. The methanol sensing application of the H_2SO_4 doped PmAP was carried out, which showed an increase in conductivity under the flow of methanol vapor air mixture. Hence developed processable conducting polymer can be utilized in gas sensor and other instruments related to sensing. Plausible mechanism of doping of PmAP by H_2SO_4 is given in scheme 1.

Keywords: Gas sensor; conducting polymer; poly (m-aminophenol); characterization



Scheme 1. Doping of PmAP with sulfuric acid

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PP-39

Heterogenized materials as functional model for phenoxazinone synthase enzyme

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Four new dioxidomolybdenum(VI) [$Mo^{VI}O_2L^{I-IV}$] complexes based on H_4dfba(bhz)$_2$ (**I**), H_4dfba(fah)$_2$ (**II**),H_4dfba(nah)$_2$ (**III**), and H_4dfba(inh)$_2$ (**IV**) ligands (H$_2$dfba = 3,5-diformyl-4-hydroxybenzoic acid, Hbhz = benzoylhydrazide, Hfah = 2–furanoylhydrazide, Hnah = nicotinoylhydrazide and Hinh = isonicotinoylhydrazide) have been synthesized and their corresponding heterogenized complexes [$Mo^{VI}O_2L^{I-IV}$]@APTMS-TiO_2 supported on amine-functionalized titanium dioxide (APTMS-TiO_2) have been isolated and characterized by various spectroscopic techniques (FT-IR, UV-Vis, diffusion reflectance, ^{1}H and ^{13}C NMR), elemental analysis, thermal, TEM and powder X-ray diffraction studies. Single-crystal X-ray study of [$Mo^{VI}O_2${H_2dfba(bhz)$_2$}(EtOH)] (**1**) and [$Mo^{VI}O_2${H_2dfba(nah)$_2$} (EtOH)] (**3**) confirms the octahedral structure. Both homogeneous and heterogeneous complexes have been explored as phenoxazinone synthase mimicking catalysts in the oxidation of 2-aminophenol to 2-aminophenoxazine-3-one in acetonitrile in the presence of aq. H_2O_2. The k_{cat} value for the phenoxazinone synthase-like activity was found to be 1.46×10^{-3} and $3.26 \times 1\ 0^{-3}$ min^{-1} for catalysts **1** and **2**, respectively. All the catalysts yielded 2–aminophenoxazine-3-one (APX) in the range of 86–94 % under the optimized reaction conditions.

Keywords: Dioxidomolybdenum (VI) complexes; Heterogeneous catalysis; Single-crystal X-ray diffraction studies; Oxidative coupling of 2-aminophenol; phenoxazinone synthase activity

PP-40

Highly Selective Fluorometric Sensing of $H_2PO_4^-$ By Using a Benzothiazole Based Receptor with Real Sample Analysis and ATPase Activity Profiling

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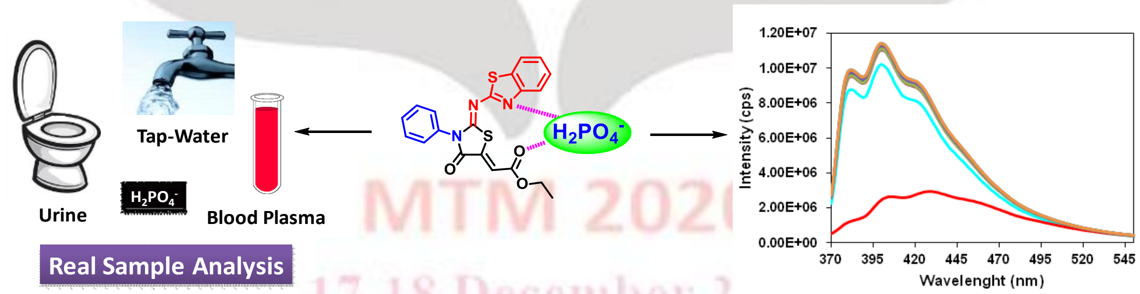
A new fluorescent chemosensor (*Z*)-ethyl 2-((*Z*)-2-(benzo[d]thiazol-2-ylimino)-4-oxo-3-phenylthiazolidin-5ylidene) acetate (receptor **1)** was designed, synthesized and applied for the detection of bioactive anions. Receptor **1** was built on the basis of internal charge transfer (ICT) mechanism with benzothiazole unit, and the results are complemented with density functional theory (DFT) calculations. In CH_3OH/ H_2O (50:50, *v/v*) medium, the emission of receptor **1** is quenched significantly in the presence of $H_2PO_4^-$ among the other tested anions (F^-, Cl^-, Br^-, I^-, CH_3COO^-, NO_3^-, CN^-, HSO_4^-, HSO_4^- and biomolecules like ATP, AMP, NADP, NADH and NAD). It is proposed that Receptor **1** forms complex in a 1:1 stoichiometry with $H_2PO_4^-$ and its detection limit is found to be 0.17 μM. In addition, the sensor was successfully used to investigate the analytical concentration level of $H_2PO_4^-$in blood plasma, urine as well as tap water samples. As a final point, the fluorescence profiling successfully monitoring on ATP in lysosomes by apyrase enzyme.



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KEYNOTE SPEAKERS

KN-01

Ashok Kumar Mishra, IIT Madras, INDIA

Professor Ashok Kumar Mishra completed his Master of Science from University of Delhi in 1980 and received PhD from IIT Kanpur in 1985. After a stint in Sambalpur University as a faculty member, and in Gunma University (Japan) as a Monbusho fellow, he joined IIT Madras in 1992. He was a JSPS Visiting Scientist in Gunma University, Japan during 2002-2003. Currently he is working as Professor in the Department of Chemistry, IIT Madras. He also handles the responsibility of Dean Academic Research at IIT Madras. Prof Mishra is a Fellow of the 'National Academy of Sciences, India'. Awards received by him include 'CRSI Bronze Medal' from the Chemical Research Society of India, 'Acharya P C Ray Memorial Award' from Indian Chemical Society and 'Prof W U Malik Memorial Award' from The Council of Chemists.Prof Mishra works in the general area of *Physical Photochemistry* and *Fluorescence Spectroscopy*. He has an active research group. So far he has guided 27 PhDs, many M.Sc. students, and published about 210 research papers, reviews and monographs.

KN-02

Shin-ichi Yusa, University of Hyogo, JAPAN

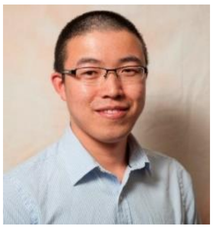
Professor Shin-ichi Yusa is a native of Japan and received B.S. (1993) and M.S. (1995) degrees in polymer chemistry from Osaka University under the direction of Prof. Mikiharu Kamachi and Prof. Yotaro Morishima. He received a Ph.D. from Osaka University (2000) for a thesis entitled: "Synthesis of Cholesterol Bearing Polymers and Their Self-Assembling Properties." He joined Himeji Institute of Technology as an assistant professor in 1997. He became associate professor of University of Hyogo (2008). His research interests are in controlled radical polymerization and characterization of water-soluble polymers. He is currently on Associate Editor of Polymers (MDPI Publishing) and Editorial Advisory Board of Langmuir (ACS). He is also on the editorial board of E-Journal of Chemistry (Hindawi Publishing), Open Journal of Polymer Chemistry (Scientific Research Publishing), and Open Chemistry (DE GRUYTER).

KN-03

Kuruvilla Joseph, Indian Institute of Space Science and Technology, Thiruvananthapuram, INDIA

Professor Kuruvilla Joseph is the Outstanding Professor & Dean, Indian Institute of Space Science and Technology. Prof. Kuruvilla Joseph has been listed among the top 2 percent scientists (rising stars), by Stanford University, across the world in all subject fields. His H Index is 52, and i10 index is 155. He has more than 11800 citations to his credit. Besides he has published four academic books by international publishers as author / editor and published more than 25 book chapters and has been invited as speaker for hundreds of National and International Conferences. He has 3 patents and more than 200 publications in international journals. The academician has produced 20 Ph.D.s and several Master Projects. Choice of research areas include Nanomaterials and Nanocomposites, Polymer Blends and Composites, Synthesis of polymers from natural resources, Green materials and bio-composites, ageing and degradation and development of biosensors. Prof Joseph has also been honoured with Linnus-Palme Visiting Scientist Fellowship, Sweden, the DST (India)-DAAD (Germany), Visiting Scientist Fellowship, Martin Luther University, Halle, Germany, the Visiting Researcher Fellowship of Swedish Institute of Composites (SICOMP), Sweden, the Visiting Professor Fellowship of the National Council for Scientific and Technological Development (CNPq), Govt. of Brazil, the Visiting Researcher Fellowship of Indian National Science Academy(INSA), New Delhi and the Research Associateship of the Council of Scientific and Industrial Research (CSIR), Govt. of India, New Delhi.

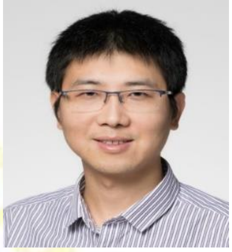
KN-04



Run Zhang, The University of Queensland, AUSTRALIA

Run Zhang received his PhD from the Dalian University of Technology in 2012. He was a Postdoc Research Fellow at the Department of Physics and Astronomy in Macquarie University (MQ) in 2012, then a Macquarie University Research Fellow at the Department of Chemistry and Biomolecular Science in 2013-2015. He joined the Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, as a Research Associate in 2016. Here, he was awarded the Australian Research Council Discovery Early Career Researcher Award (ARC DECRA) Fellowship in 2017-2019 and is now a National Health and Medical Research Council (NHMRC) Emerging Leadership Fellow. He is currently a group leader of the biosensing and bioimaging, working on the development of responsive molecules/nanomaterials for early disease diagnosis and treatment. He has published about 110 research papers since his first publication in 2010.

KN-05



Prof. Y. Bao, Department of Chemistry and Applied Biosciences, SWITZERLAND

Yinyin Bao received his bachelor degree in Macromolecular Materials and Engineering (2007) from Hefei University of Technology and PhD degree in Polymer Chemistry (2012) from University of Science and Technology of China. From 2012 to 2014 he completed a postdoctoral research at KU Leuven (Belgium), and then became a Marie Curie Intra-European Fellow in the French National Center for Scientific Research (CNRS) at University of Paris Sud. From 2016 he joined the group of Prof Jean-Christophe Leroux at ETH Zürich, and he was promoted to a Senior Scientist position as a group leader at the end of 2018. Dr. Bao in currently leading a highly interdisciplinary project funded by Swiss National Science Foundation (SNSF) about 3D printed biodegradable personalized medical devices (Sinergia, 2.3M CHF), in collaboration with three different groups at ETH Zürich, University of Zürich and University Hospital Zürich. He is also a principal investigator for two research projects about modulation of molecular fluorescence in solid state by precision macromolecular engineering, which are funded by Foundation Claude et Giuliana (144K CHF) and SNSF (100K CHF). His research interest remains the application of polymer chemistry in biomedical area, such fluorescent sensing and imaging, drug delivery, 3D printed medical devices, etc. He has published more than 30 scientific papers and 1 book chapter with H-index of 18 and citations > 1000. He serves as a founding member of Sounding Board of Competence Center for Materials and Processes (MaP) at ETH Zurich from 2020.

KN-06

Ajay Kumar Dalai, University of Saskatchewan, Canada

Professor Ajay Dalai is a Canada Research Chair *in Bioenergy and Environmentally Friendly Chemical Processing* in the Department of Chemical and Biological Engineering at the University of Saskatchewan. He obtained his B.Tech degree from LIT Nagpur and M.Tech degree in Chemical Engineering from IIT Kanpur and then his PhD degree in Chemical Engineering from the University of Saskatchewan. With PDF experience at Texas A&M University and University of Calgary, he started his career with the University of Saskatchewan in 1996 as Assistant Professor in the Department of Chemical Engineering, with promotions to Associate Professor in 1998 and to Full Professor in 2002. His research focus is the novel catalyst development for gas to liquid (GTL) technologies, biomass utilization, biodiesel production and applications, hydrogen/syngas production from waste materials, hydroprocessing of heavy gas oil, and value-added products from biomass, production and applications of activated carbon and carbon nanotubes (CNTs), and utilization of micro-algae for fuels and value-added bio-products. He is a lead user of synchrotron radiation facility at the University of Saskatchewan. Dr. Dalai has filed several patent applications and has published over 490 research papers in international journals and conference proceedings and books, mostly on heterogeneous catalysis and catalytic and green processes, with citations over

23,000 and H-index of 73. Dr. Dalai is an active board member, reviewer, and guest editor for several international journals. He is honoured as a *Fellow of the Canadian Academy of Engineering*, a *Fellow of the Chemical Institute of Canada, Fellow of Engineering Institute of Canada, Fellow of American Institute of Chemical Engineers and Fellow of Indian Institute of Chemical Engineers, Fellow of Royal Society of Canada, Fellow of Royal Society of Chemistry (UK)*, a *USA Fulbright Fellow*, a DAAD Fellow and JSPS Fellow, Most recently, he gave seminars at the Universities of Edinburgh, University of Aberdeen, Harriot-Watt University, Imperial College and Cambridge University as part of the Royal Academy of Engineering fellowship in UK. In January 2020, Professor Dalai is appointed as *Distinguished Professor* at the University of Saskatchewan.

KN-07

Qianqian Su, Shanghai University, Shanghai , People's Republic of China

Qianqian Su received her BE degree from Shandong University. She received her MS degree from Guangzhou Institute of Chemistry, Chinese Academy of Sciences and completed her PhD degree under the supervision of Professor Xiaogang Liu at National University of Singapore. She worked as a research fellow at Fudan University with Professor Fuyou Li. She then worked as a visiting scholar at National University of Singapore, University of Technology Sydney and Genome Institute of Singapore. She joined Institute of Nanochemistry and Nanobiology at Shanghai University in 2017. Her research interests focus on the development of novel luminescent nanomaterials for biomedical applications. Dr. Su has authored 3 patents and 30 peer-reviewed scientific journals (total citation > 3000, Google Scholar), including *J. Am. Chem. Soc.*, *Adv. Mater.*, *Nat. Commun*, *Acc. Chem. Res*, etc., 6 of which were selected as Highly Cited Papers in ESI.

KN-08

Pil Seok Chae, Hanyang University, South Korea

Pil Seok Chae is a professor at Department of Biotechnology, Hanyang University, South Korea. He did PhD from Deoul National University in 2006 and worked as a research associate at University of Wisconsin, (UW-Madison) from 2006-2011. He has over 99 publications in high quality journals and received several awards and fellowship like University ERICA Academic Research Award (2018), LG Yonam Fellowship (Overseas Research Professor)(2018) Best teacher of Hanyang University (2014, 2015) and POSCO Science Fellowship (New Faculty)(2014). His main research area includes membrane protein extraction, stabilization and crystallization, protein-detergent interaction.

KN-09

Gopinath Sankar, University College London, UK

Professor G Sankar obtained his PhD from Indian Institute of Science, Bangalore in 1987. He was elected as the Young Associate fellow of Indian Academy of Sciences in 1988 for his contribution to X-ray spectroscopy. He joined the Royal Institution of GB in 1990 where he held several positions, which includes PDRA, Assistant Director of DFRL, Leverhulme Senior Research Fellow. He became Professor of Solid State Chemistry in 2004, at the Royal Institution and moved to Department of Chemistry, University College London, in 2007 where he continue his research in the following areas. His research group have been involved in the study heterogeneous catalytic materials. In addition, his group uses advanced Synchrotron Radiation techniques to investigate formation catalytic materials, structure of these catalytic materials at various length scales. His research focusses on the determination of structure function relationships. Sankar was awarded a Royal Society Industry Fellowship to carry out collaborative research with Johnson Matthey plc. and he continue to closely work with scientists at Johnson Matthey. He has supervised over 40 PhD and Post-Doctoral researchers. He has over 275 publications and his current H-index is 59 with overall citations over 11000.

KN-10

Reza, Sharif University of Technology, Iran

M. Reza Hormozi-Nezhad is a Professor of Analytical Chemistry at the Chemistry Department and Director of Research at Sharif University of Technology. His research interest mainly includes sensing and biosensing based on plasmonic and luminescent nanoparticles (NPs), and developing nanostructure-based optical sensor arrays for the determination and discrimination of important chemical and biological active compounds.

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